



Introduction

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Trends and challenges in the mechanics of complex materials: a view

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This article introduces the collection of papers in this issue of the *Philosophical Transactions of the Royal Society A* and offers a perspective view on the description of the mechanics of material characterized by a prominent influence of small-scale phenomena on the gross mechanical behaviour.

1. Preamble

This article places the papers collected in the present miscellanea in a panorama on the continuum mechanics of materials. Introducing these articles does not require a big effort from my side because the contributions sustain themselves with their evident quality. The difficulty that I find is essentially in presenting a rather broad view on the research paths in continuum mechanics, which is the other aim of this paper, as required by the Editorial Office in assigning me the editorship of this issue. The enterprise faces the limitation of my knowledge and my personal view on what I believe are essential aspects of the landscape that I want to delineate. For this reason, the view that I offer is neither complete nor neutral; but it is a view in any case and may help the patient reader to form a personal opinion, even in opposition.

2. Some sparse historical notes on mechanics with special attention to continuum schemes

Mechanics is the body of speech about the description of motions of objects at human, microscopic, giant scales, even at the scale of the universe. We distinguish among the motions of mass points, multi-particle systems, rigid and deformable bodies, and subatomic particles. We then speak about classical, statistical, continuum, relativistic, quantum mechanics, kinetic theory, subdividing the subject into sectors in accordance to classes of phenomena and/or descriptive tools.

However, looking at the foundational issue, which is concretely different from being interested merely in the formal structure of theories, as even an elementary education in philosophy allows us to distinguish, we realize in the end that these sectors are not disjoint, rather they fertilize each other and sometimes we try to show that a viewpoint is the limit in some sense of another view. Examples in this vein are the analysis concerning the limit of the Boltzmann equation when the number of particles increases to infinity (recall: the equation describes the evolution in time of the distribution function of velocities of several, but finite in number, mass points, possibly colliding with each other) or the atomistic-to-continuum schemes proposed in materials science often on the basis of density functional theory: an approximation of quantum mechanics.

In the *Prefatio ad lectorem* of the *Philosophiae Naturalis Principia Mathematica* [1], Isaac Newton recalled the subdivision of the mechanics by his predecessors into rational (*rationalem*) and empirical (*practicam*). The former proceeds in terms of rigorous proofs (*quae per demonstrationes accurate procedit* in the original version), expressed in mathematical terms. The latter deals with the construction of machines and tools useful for everyday life. Both views cross-fertilize and are not distinguished, although single scholars can emphasize one in contrast to the other, often instrumentally, to defend their own position. The same design of an experiment foresees a preliminary, even vague, theoretical view on a phenomenon that we want to reproduce and measure. In turn, an acceptable theoretical proposal must adhere to the pertinent phenomenology that we record.

Newton's view on mechanics was eminently geometrical. In the first part of the *Prefatio*, he remarked that geometry emerges from mechanics. Only 63 years after the publication of the *Principia*, Leonhard Euler wrote the second law of motion, the balance of momentum, in the differential form that we use today, in an article entitled *Decouverte d'un nouveau principe de mécanique*, read in front of the Berliner Academy on 3 September 1750, and published 2 years later [2]. The balance of the moment of momentum, which is not explicitly discussed in Newton's *Principia*, appeared in a 1703 article by Jakob Bernoulli [3]. Newton's *Principia* evidenced problems and techniques, had a decisive impact on the development of the scientific thought and opened a path along which rational mechanics developed systematically. Newton's viewpoint indicated new territories both in the norms adopted to explain concepts and in the mathematical techniques, but already the ancient Greeks had the perception of the vastness of the subject. In fact, the oldest text on mechanics that we know of is in Greek: *Mechanical Questions*. Historians still debate whether we have to attribute it to Aristotle (384–322 BC), Archytas of Tarentum (428–347 BC), or even and more generically we can affirm it has been written by some fellow of the Lyceum in Athens to interpret some phenomena in the terms of Aristotelian natural philosophy [4]. The list of topics discussed in *Mechanical Questions* includes cases that can be analysed by considering the scheme of rigid bodies and also cases where strain plays a prevalent role, as in the discussion of vorticity in fluids there included.

The idea that the language of mechanics in its theoretical development must be analytical appears explicitly in the title of the treatise on mechanics that Euler published in 1736, after having completed it, at 27 years old, in his first period in San Petersburg [5]. Later, in his *Cours de Philosophie Positive*, 1830–1842, Auguste Comte emphasized the rational aspect of the approach to mechanical problems and the status of rational mechanics as an independent discipline [6]. However, although the foundations of mechanics can be expressed just in analytical and geometrical terms, their essence is in the connection with the phenomenological world.

Already in the first treatises on mechanics, we find questions that are still contemporary for they deal with the nature of the subject and its mathematical structure. They include discussions on the nature of the basic principles and their explicit expressions in specific contexts, the way in which we describe bodies and what we consider to be a body, the representation and the nature of the interactions among portions of a body and with the surrounding environment, etc. Statements such as 'forces are, in mechanics, no more than the movements produced, or going to be produced [*virtual* in modern terms; *my note*], and two forces which induce the same velocity in the same direction are considered identical, their origin whatever ...' that we find in Comte's *Cours* (*Cours, quinzième leçon*, tome I, p. 544) fall completely within the modern view on interactions defined

by the power that they develop, being represented by entities dual of what describes the rate of change of the body morphology (in geometric terms, they are elements of the cotangent space of the manifold describing the body morphology; e.g. [7]). This abstract view allows us to go into a rather secure path when we want to describe circumstances requiring a geometric setting more complicated than the standard three-dimensional Euclidean point space equipped with a single Cartesian frame. I shall provide pertinent examples.

Rational mechanics is part of mathematics not so much for what the adjective ‘rational’ recites as for its structure and the methods pertaining to it. This is evident if we look at it from the interior, above all having a creative daily frequentness with it, not forgetting to take into account the diversity of the results in mechanics, in nature and quality. Following the ramifications of mechanics, those listed in beginning this section, with the aim of offering a comprehensive view on them, is an arduous task even for a ponderous treatise, but it is also so even when we restrict ourselves to a single subfield, as I do here, focusing the attention on continuum mechanics of condensed matter, because it allows us a view in which we find a perspective of the various ramifications of mechanics that emerged in time from the first results on the matter. On one side, continuum mechanics of materials calls upon concepts and classical issues pertaining to the mechanics of mass points and rigid bodies. On the other side, it pays attention to a more and more detailed description of materials, some constructed anew to satisfy peculiar technological needs. In its edge developments, continuum mechanics involves concepts from and establishes links with statistical and quantum theories, proposing itself as a favourable playground for a general discussion on the nature of mechanical models and the role of mathematics in mechanics.

The standard format of continuum mechanics, initiated primarily with the works by Euler, Bernoulli and Augustin Louis Cauchy, has been axiomatized in the second half of twentieth century by the original nucleus of Clifford Ambrose Truesdell’s school, starting with the 1958 seminal article by Walter Noll [8].

The basic question raised in the mechanics of bodies undergoing strain is intuitive: consider a generic object of sensory perception, a tangible body with dimension greater than the atomic ones and smaller than the scale of the universe. Take it in some shape, which we consider as a reference, and try to determine how the body shape changes as a consequence of the interaction with the external environment. The consequent analysis implies descriptive choices before tackling analytical and geometrical difficulties. The rational character of the approach manifests itself in the way we articulate the initial choices.

- The starting point is geometric: we need to specify in some way the shape of a body that we consider undeformed, because measuring strain means evaluating how lines, volumes, areas vary within a body under the action of the external environment. About this first step, the traditional format of continuum mechanics (see basic treatises on the matter, [9–14]) shows a minimalist approach: we describe the shape of a body by selecting just the fit region in three-dimensional space it may completely occupy, without adding any geometric information on the way the matter is arranged at microscopic scales. Every point of such a region is intended as the place of what we call a *material element*, a conglomeration of atoms, an indistinct mass point endowed just with 3 d.f. in Euclidean point space.
- Such initial choice determines the description of the interactions among distinct parts of the body and the external environment. Subdivided into bulk and surface actions, they are defined as elements of the dual space of what describes the rate of change of the body morphology, as I have already mentioned, and satisfy the balance equations, which may originate from multiple sources. The investigation of the nature of their origins is essential for the individuation of reliable paths to determine them when we want to build up new models. In fact, acting in analogy with well established practice, e.g. the balance equations pertaining to a single mass point or a rigid body subjected to the action of the external environment, may be at times just a hope to determine the result. The more we know

- about the nature of the interactions on and in a body, the more we can be sure about the identification of the appropriate balance equations.
- Then we furnish information (indirectly in a sense) on the essential aspects of the material structure through the *state functions*, the so-called *constitutive relations*, which link what we have selected as state variables (another modelling choice) to the interactions within the body under analysis. Experimental data address the selection but there is certain arbitrariness in the choice. The second law of thermodynamics and the requirement that the structure of the physical laws should not change under changes in observers impose *a priori* theoretical restrictions on the possible constitutive choices. The decision to adopt these constraints is philosophical and requires some concepts to be specified. We need, in fact, to clarify what kind of expression of the second law we consider. We also find it necessary to define the nature of the observers (and the one of observable quantities) and the classes of their changes.
 - In classical mechanics, an observer is a frame in the ambient physical space and a time scale. Once we assign it, we impose some basic elements of our models *objectivity*, i.e. invariance with respect to rigid-body-type changes in observers, or *covariance*, which involves non-rigid changes of coordinate frames in space. These requirements determine non-trivial consequences. For example, in the description of the (isothermal) elastic behaviour of bodies called *simple* for their energy depends only on the first spatial derivative of the deformation, in the presence of large strains the requirement of objectivity for the energy (two observers differing by a rigid-body motion must evaluate the same internal energy of the body under analysis) implies the physical incompatibility between the objectivity itself and the possible convexity of the energy with respect to its entry, the sole state variable considered in this case. Such a result has given further impulse to the whole sector of the analysis of polyconvex functionals in the calculus of variations [15,16].
 - Besides restrictions due to the second law and the requirements of objectivity or covariance, constitutive equations are essentially phenomenological. A question is then whether atomistic descriptions of the matter can justify at least classes of state functions. The question emerges from the desire of reducing as much as possible the introduction of phenomenological parameters, which may have uncertain values, even origin. Already Cauchy tackled the question with the aim of interpreting in atomistic terms the constitutive relations of the linear elasticity. He considered a discrete structure constituted by mass points and linear springs. His idea was to try to transfer the properties of the discrete structure, a scheme of a crystalline body, in a continuum representation. A debate between the so-called molecular interpretation of elasticity and the phenomenological approach animated that period and overrode it eventually [17]. At least for crystalline materials, an essential element clarifying the link with the molecular approach emerged from Max Born's work and is what we call today the Cauchy–Born rule [18]. Cauchy assumed coincidence between macroscopic and atomic movements, while Born modified the view presuming that the lattice vectors of a deformed crystal are the image of those in the reference crystal though the macroscopic deformation gradient. In his view, the characteristic cell of the crystalline lattice undergoes a homogeneous strain. For two-dimensional mass-spring lattices, the Cauchy–Born rule is actually a rigorous theorem for an open set of model parameters (equilibrium lengths and spring constants) for all boundary data close to the identity, while it fails for another open set of parameters [19]. Fine scale spatial oscillations appear in that parameter region in the energy-minimizing configurations. On the other hand, atoms are rather complicated structures. Viewing them as mass points is an idealization, which has, however, its possible justifications in the circumstance that, at zero temperature, a canonical ensemble becomes a degenerate distribution and localizes on (discrete) minimizers of the energy. And this is a result of statistical mechanics. Moreover, since elastically deformed states are in general just local minimizers of the energy, we can show that the Cauchy–Born rule is always valid for

elastically deformed crystals, provided appropriate choices of the unit cell characterizing lattice periodicity [20,21]. The idea underlying the Cauchy–Born rule can be generalized to multiple lattices [22] or to an expression in terms of velocities. Such a rule, however, is not the unique link between continuum and corpuscular descriptions of the behaviour of the matter. I have already mentioned at the beginning of this section the question of the continuum limit of the Boltzmann equation [23]. We can list other relations between continuum and quantum multi-body schemes and we welcome these connections for they do not contain empirical parameters (an example is the scheme to get a continuum model of thin films from the superposition of mono-atomic lattices [24]). Nevertheless, the complexity of the approaches requires non-trivial approximations, which can even account for inhomogeneous electron systems. The Thomas–Fermi method, which is valid when the spatial variations of de Broglie’s wavelength are small, is in this vein. So is Slater’s simplification of the Hartree–Fock equation. It is based on the expression of the wave function of a system of N interacting particles in terms of a matrix with entries orthogonal wave functions of single particles. Kohn’s & Sham’s theory [25] enlarged the setting. It has its roots in Thomas–Fermi’s theory (e.g. [26]) and refers to quantum systems involving many bodies. It rests on the choice of a non-local energy, but the exchange potential, which accounts for all the interaction effects among the bodies considered, has local nature. Under appropriate conditions, the equation emerging from the first variation of the energy considered by Kohn and Sham admits locally unique solution, which can be well approximated by using a version of the Cauchy–Born rule [27]. We recover this way the link between continuum and atomistic approaches.

Beyond the interactions with quantum or statistical descriptions, the same internal structure of continuum mechanics should be flexible to describe even unexpected expressions of condensed matter. Reasons for this need emerge from specific circumstances.

3. What pushes us towards and beyond the borders of the traditional format of continuum mechanics of materials

In summary, the traditional format of continuum mechanics in classical space–time, as sketched in the previous section, is based on a conceptual hierarchy:

- (i) representation of the morphology of a body (its geometrical description), which is traditionally restricted to a region in space that can be occupied by the body under analysis;
- (ii) representation of the interactions with the environment and inside the body, essentially a consequence of the first item and statement of the pertinent balance equations; and
- (iii) assignment of the constitutive structures.

A common, instinctive tendency is to consider the construction of a model in continuum mechanics as coincident *only* with the construction of an appropriate constitutive relation, i.e. a functional structure linking state variables with the stress, leaving as granted once and for all the description of the body’s morphology and the representation of the interactions, with their related balances. This view is often satisfactory but in non-trivial circumstances it can be considered at least short of breadth. Just to solicit the reader’s imagination, an incomplete list of pertinent cases follows:

- Liquid crystals are composed of stick molecules with end-to-tail symmetry, which self-organize aligning some way, driven by the interaction with the environment. A geometric need is then the description of the local orientation of the molecules, because it determines the essential peculiarities of liquid crystals, i.e. the transition from an order of

- alignments to another. The standard deformation map does not bring such information. Moreover, the alignment of the stick molecules involves interactions not easily ascribable to the standard traction due to deformation.
- When strain, temperature, external electric fields overcome some threshold, ferroelectric materials undergo polarization, while magnetoelastic solids show local magnetization. Stretchable vectors up to a certain limit length describe locally the polarization. Peculiar bulk and contact interactions are pertinent to (in the sense that they develop power in) the time rate of the polarization. Their description falls outside the standard scheme indicated by Cauchy's stress tensor.
 - The motion of dislocations in metals, the occurrence of slips in crystals or among grains in an amorphous solid, the creation of micro-voids are sources of what we call elastic-plastic behaviour. In describing it, we can look just to the macroscopic measure of irreversible strain by introducing F^p , the plastic factor of the deformation gradient F in a multiplicative decomposition, with the related measures of deformation, and at times even its spatial derivative in the so-called second-grade (or strain-gradient) approaches to plasticity. Alternatively, we can have a close look to the microscopic mechanism, considering, e.g., peculiar descriptors of the slip velocity or the dislocation density, or something else that we consider essential in representing the roots of the phenomenon in the microscopic world. The paper by Irene Bayerlein and Abigail Hunter and the paper by Gareth Parry in the present miscellanea show possible views on the problem and different descriptive choices. In this case, the scenario of the interactions occurring within the body and with the rest of the environment becomes more rich than the standard one and we can, e.g., investigate the microscopic origin of concepts, such as the back-stress, e.g., otherwise introduced just phenomenologically, often on the basis of data-fitting approaches.
 - Bones show an intricate microstructure, which we can call 'trabecular' or spongy. Local alterations of this structure, such as the occurrence of microcracks or local instabilities, may cause damage. Their description goes beyond the standard continuum mechanics view. So it is for other biological materials.
 - Phase transitions of the first and second kind require at least the information on the volume fraction of the transforming phases, besides the standard deformation, when we do not need more refined description of the way matter changes its state. Clear examples of possibilities appear in the contribution by Yaniv Ganor, Traian Dumica, Fan Feng and Richard D. James and the one by Thomas J. Pence and Davide Bernardini in the present miscellanea.
 - Damaging a solid is a relative concept: we have to define a state that we consider undamaged. Damage is a word used to indicate the result of different processes: microcrack evolution, void nucleation, corrosion, ageing. With respect to processes, damage is a collective word, in this sense. A question is how to describe a damaged state and its possible evolution. There are various possibilities, which can be subdivided in two different classes: we use variables measuring the removal from thermodynamic equilibrium, whatever the damage mechanism be; we introduce variables bringing geometric information on a specific mechanism generating damage. The paper by Christian Miehe, Stephan Teichmeister and Fadi Aldakheel, in this issue, indicates an intricate, although clear, possibility of describing the coalescence of damage up to the creation of a macroscopic crack. In any case, the question of the nature of the supplementary variables is more general so that at least a vague tendency towards completeness or a reasonable deepness forces me to return to this matter later on.
 - Composites made of polymers scattered in a melt with different stiffness may suffer relative strain of the added molecules with respect to the melt. We need then a second-rank tensor describing the molecular strain, a micro-strain because it is at a spatial scale smaller than—let us say—the one of human naked-eye observation.
 - Polymeric chains can be ordered in measures resembling the order of liquid crystals. Polymers can be also of star-type so that we have to add information on the diameter of

the molecular part rolled into a ball. Also they can suffer polarization. From a geometrical viewpoint, the deformation alone is not sufficient to describe these microscopic features and appropriate descriptors have to be inserted. So it is for other offspring of condensed matter as quasi-crystals or the superfluid liquid helium.

- Quasicrystals are aluminium-based alloys characterized by quasi-periodic arrangements of atoms. The representation of their mechanics involves deformation but also the need of describing at macroscopic scale local phase changes in the symmetry of the atomic arrangements, due to flips of atoms, which are necessary to match quasi-periodicity under the action of the external environment.
- Superfluid liquid helium shows different microscopic features in accordance to its particular phase. We can need a number selected in the unit circle in the complex plane or an orthogonal tensor with positive determinant, an element of $SO(3)$ then.
- We can have cases in which not so much the inner material structure of a body as the smallness of one of its characteristic dimensions determine a peculiar behaviour. This is the case of shells, above all thin films, and their interactions with the surrounding environment, as evidenced, e.g., in the paper by Nicholas Brubacker and Joceline Lega in this miscellanea.

All the examples above are related to cases in which events developing at very small spatial scales with respect to the size of the body have influence on the macroscopic mechanical behaviour, exerted through interactions barely representable in terms of standard stresses. We can call *complex materials* those characterized in this way to remind these peculiarities.

The effects of the microstructural changes can be at times described even within the traditional setting as ‘irregularities’ of the deformation. Even in this case, however, we need to often render evident the scaling, as shown in the paper by Likun Tan and Kaushik Bhattacharya in the collection of contributions here introduced.

In any case, in constructing a continuum model of deformable bodies we need to take a decision already from the first step in the hierarchy presented above, i.e. the representation of the morphology of a body. Adopting the standard minimalist view, which requires for a body just the selection of a fit region in space, is a choice. It can be enriched by the addition of variables carrying information about the way the matter is arranged or the features involved in a class of specific phenomena, as in the cases summarized in the items above. A basic question is to decide whether the variables that we may introduce besides the deformation have just the role of measuring, at a stage subsequent the description of the body morphology, the removal of the body from thermodynamical equilibrium (as in [28–31]), or they furnish information on the body geometry and are sensitive to changes in observers (as in [32]). In the first case, we do not need to specify the physical nature of the variables introduced and we assign essentially *a priori* their evolution, so that we speak about *internal variables*, according to the common jargon introduced first in non-equilibrium thermodynamics [33] and then coupled with deformation later in the references already mentioned. In the second case, we are introducing explicit direct or indirect information on the shape that the body can have, expressed by variables that may be sensitive to changes in observers just for this reason. Such variables can be associated with a distinguished specific geometrical feature or may emerge from some statistical analyses, which may also allow us to homogenize the material heterogeneity to get an ‘equivalent’ traditional continuum by exploiting even intricate aspects of the stochastic calculus, as indicated in the paper by Xavier Blanc, Claude Le Bris and Frederic Legoll in this collection of research contributions. Moreover, the change in the geometric descriptive setting imposes us to think again of the notion of observer. The distinction between the two ways of considering additional variables (see also relevant discussions in [34]) has non-trivial physical consequences. In the first case, just thermodynamic affinities are associated with the rate of change of these variables and they contribute just to dissipation, while they play a parametric role at equilibrium, along conservative processes. In the second case, we find true interactions, which satisfy appropriate balance equations. However, formally the first case can be included in the second one, but the conceptual difference remains.

The resulting models propose even arduous mathematical questions, as it emerges, e.g., from the article by Sebastian Heinz and Alexander Mielke in this collection.

Some details, above all about the general model-building framework emerging from the second viewpoint, clarify the discussion for me.

4. Morphologies

In the traditional setting of continuum mechanics of materials, a tangible body is viewed as an abstract set B of not further specified *material elements* [8]. We then imagine the possibility of establishing a one-to-one mapping

$$k: B \rightarrow \mathcal{E}$$

from B into the Euclidean point space \mathcal{E} with dimension specified by the problem at hand; typically 1, 2, 3, although to fix ideas we consider here just the three-dimensional case. In this way, we represent the set B by its image $\mathcal{B} := k(B)$ and the geometric description of a material element reduces to the assignment of a point in space.

We take \mathcal{B} as an open bounded set coinciding with the interior of its closure and presume that it is endowed with surface-like boundary oriented by the outward unit normal everywhere with the exception of a finite number of corners and edges. Maps

$$u: \mathcal{B} \rightarrow \tilde{\mathcal{E}},$$

commonly assumed to be one-to-one, differentiable and orientation preserving, allow us to define shapes of the body that we consider *deformed* with respect to \mathcal{B} . So we call u a *deformation* and write y for the value $u(x)$. The selection of a functional space for deformations is already a *constitutive assignment*. A function space is defined, in fact, by some properties pertaining to its elements, so that they may describe some peculiarities of a class of material behaviours, excluding others.

In the above definition of u , the space $\tilde{\mathcal{E}}$ is a copy of \mathcal{E} , obtained by an orientation-preserving isomorphism or more simply the identification. The distinction between the space in which we select the reference macroscopic shape of a body and the one including its deformed configurations finds its reason of being in two basic aspects: one is connected with the definition of changes in observers, the other concerns the computation of the so-called *vertical* and *horizontal* variations of the energy in the conservative case, the former leading to the balance of forces, the latter producing the balance of configurational interactions, at least in the conservative case.

At $x \in \mathcal{B}$, consider a vector basis $\{\mathbf{e}_A\}$ in \mathbb{R}^m and a scalar product $\langle \cdot, \cdot \rangle$, which determines a metric g at x , a second-rank tensor with generic component g_{AB} defined by $g_{AB} := \langle \mathbf{e}_A, \mathbf{e}_B \rangle$. g is positive definite because $\{\mathbf{e}_A\}$ is a basis and the scalar product is non-negative. Consider now the space of linear functions over \mathbb{R}^m . For \mathbf{f} and element of such a space, write $\mathbf{f}(\mathbf{e}_A) := \mathbf{f} \cdot \mathbf{e}_A$. The dual space has dimension m and its natural basis with respect to $\{\mathbf{e}_A\}$ is given by those elements, called *covectors*, indicated by $\{\mathbf{e}^A\}$ and defined by the condition $\mathbf{e}^A \cdot \mathbf{e}_B = \delta_B^A$. From now on we restrict our attention on \mathbb{R}^3 , which is obtained from the space of differences of points in the three-dimensional Euclidian space by assigning a basis and the origin of the related coordinate frame. For crystalline bodies, the assignment of the metric in the reference space, a *material metric*, as we have done so far, has a stringent physical character because the vectors $\{\mathbf{e}_A\}$ can be selected as those of the optical classes of the pertinent crystals, evidenced by experiments.

We indicate as usual by F the spatial derivative of the deformation, calculated at x . Precisely, we have $F := Du(x)$, with F expressed in components by $(\partial u^i(x)/\partial x^A)\tilde{\mathbf{e}}_i \otimes \mathbf{e}^A$, where $\{\tilde{\mathbf{e}}_i\}$ is the counterpart of $\{\mathbf{e}_A\}$ at $y := u(x)$; in the previous formula uppercase indices refer to coordinates on \mathcal{B} , while lowercase indices refer to coordinates on \mathcal{B}_a . The determinant of F allows us to formalize the intuitive request that u has to be orientation-preserving. The condition is then expressed by the nonlinear constraint $\det F > 0$. By definition, F maps linearly tangent vectors to \mathcal{B} at x onto the tangent space of \mathcal{B}_a at $y := u(x)$. To summarize this statement, we write $F \in \text{Hom}(T_x \mathcal{B}, T_y \mathcal{B}_a)$, where the subscript a characterizes as *actual*, i.e. referred to the deformed macroscopic shape, the mathematical ingredient that it characterizes; $T_x \mathcal{B}$ is the tangent space to \mathcal{B} at x . Two linear operators play then a role: the formal adjoint of F , indicated by F^*

and defined to be such that $F^* \in \text{Hom}(T_y^* \mathcal{B}_a, T_x^* \mathcal{B})$, and the transpose F^T , which is such that $F^T \in \text{Hom}(T_y \mathcal{B}_a, T_x \mathcal{B})$.

At any $y \in \mathcal{B}$, the basis $\{\tilde{\mathbf{e}}_i\}$ determines another metric, say \tilde{g} , which we can call *spatial* to emphasize even already in the terminology the difference with g . The pull-back $C := F^T \tilde{g} F$ of the spatial metric into the reference place \mathcal{B} , along the deformation, has components $C_{AB} = F_A^i \tilde{g}_{ij} F_j^B$, and is a metric too, due to the nonlinear constraint $\det F > 0$. Such a metric, also called the *right Cauchy–Green tensor*, allows us to define naturally a *measure of deformation* as a comparison between C and the material metric g ; we write in fact $E := \frac{1}{2}(C - g)$, obtaining in this way a second-rank tensor with components $E_{AB} = \frac{1}{2}(C_{AB} - g_{AB})$. We may also introduce the second-rank tensor $\tilde{E} := g^{-1} E = \frac{1}{2}(\tilde{C} - I)$, where g^{-1} is the inverse of g , with components indicated simply by g^{AB} , and I is the second-rank unit tensor, to have an expression of the strain measure more common. The version \tilde{C} of the right Cauchy–Green tensor is defined by $\tilde{C} := g^{-1} C = g^{-1} F^* g F = F^T F$, which is its standard expression.

I have stressed above the difference between the tangent space at a point of a configuration and its dual counterpart, i.e. the cotangent space (the space of linear forms over the tangent one), although, being in \mathbb{R}^3 or \mathbb{R}^m , they can be identified by each other. The choice is not dictated by the taste of rendering the matter uselessly intricate, rather to establish a parallelism with what we need introducing—as I try to do here—to give a unifying framework for classes of theories describing the mechanical behaviour of complex materials that we know, a framework allowing us to focus attention on the basic foundations of these theories more than on a proliferation of disconnected models almost similar one another. Of course, when the basis chosen in reference or actual configurations is unique and the basis itself is orthogonal, the previous expressions simplify. For example, the two metrics g and \tilde{g} link the adjoint of F with its transpose by the relation $F^T = g^{-1} F^* \tilde{g}$. When both g and \tilde{g} are the identity, i.e. $\{\mathbf{e}_A\}$ and $\{\tilde{\mathbf{e}}_i\}$ are orthogonal, the two linear operators coincide. For this reason, we continue to call F the *deformation gradient* although $\nabla u(x)$ and $Du(x)$ differ by the action of the metric, namely $\nabla u(x) = Du(x)g^{-1}$.

All the geometrical issues above summarized in this section describe the macroscopic configuration of a body and its changes, without furnishing *direct* information on the microscopic shape of the pertinent material at a certain spatial scale, the one involved in the possible phenomena characterizing a peculiar behaviour of the body under analysis. I have already listed examples of prominent special cases, indicating different possible choices of descriptors of the material microstructure. We can summarize all just by affirming that they are selected on a differentiable manifold, which we may select to be finite-dimensional.

We say that a set \mathcal{M} endowed with a topology such that for any pair of distinct elements of it we may find non-intersecting open neighbourhoods containing them separately is a *topological manifold* when it is *locally Euclidean*, i.e. every $v \in \mathcal{M}$ has an open subset of \mathcal{M} , $\mathcal{U}(v)$, containing it, such that it is possible to define a one-to-one mapping $\varphi: \mathcal{U} \rightarrow \mathcal{V}$ onto \mathcal{V} , an open subset of \mathbb{R}^n . We call a *coordinate chart* (simply *chart*) the pair (\mathcal{U}, φ) and an *atlas* a set $\mathfrak{F} := \{(\mathcal{U}_i, \varphi_i)\}$ of charts covering the whole \mathcal{M} . In particular, we affirm that \mathcal{M} has dimension n when all \mathcal{U}_i are mapped onto sets $\mathcal{V} \subseteq \mathbb{R}^n$ with dimension n . If for all i, j , the change of coordinates between pairs of charts is of class C^k , we say that \mathcal{M} is a *differentiable manifold of class C^k* , simply a *differentiable manifold* when $k = +\infty$. A function $f: \mathcal{J} \rightarrow \mathcal{M}$, with \mathcal{J} some interval in \mathbb{R} , defines a curve over \mathcal{M} . By definition, f is differentiable near $s \in \mathcal{J}$ when, with (\mathcal{U}, φ) a chart around $v(s)$, the map $\varphi \circ f$, with \circ indicating map composition, is differentiable in the common sense. The derivative of the function f at s is what is called the *tangent vector* to v at \mathcal{M} . The set of all tangent vectors to \mathcal{M} at v , indicated by $T_v \mathcal{M}$, and called the *tangent space* of \mathcal{M} at v , is a linear space. The union, varying v in \mathcal{M} , of all tangent spaces of \mathcal{M} is called the *tangent bundle* of \mathcal{M} and in general is not a linear space. For any $T_v \mathcal{M}$, the set of all linear functions over $T_v \mathcal{M}$ is indicated by $T_v^* \mathcal{M}$ and called the *cotangent space* of \mathcal{M} at v (its elements are commonly called *covectors*, as already recalled). The union of all cotangent spaces of \mathcal{M} is its *cotangent bundle* and is not necessarily a linear space. \mathcal{M} is rather general but it is just what we need to speak of the structure of models for complex materials constructing a unified view on the matter, at least for the cases in which we

find necessary to go beyond the standard format of continuum mechanics, except circumstances in which resort to infinite-dimensional spaces of descriptors appears necessary.

To describe specific (geometric) features of the structure of the matter at finer spatial scales, transferring them at continuum (macroscopic) scale, we define a differentiable field $x \mapsto \nu := \tilde{\nu}(x) \in \mathcal{M}$. We call it the *morphological descriptor map* and indicate \mathcal{M} as the *manifold of microstructural shapes*. We write N for its spatial derivative $D\tilde{\nu}(x)$, i.e. $N \in \text{Hom}(T_x\mathcal{B}, T_\nu\mathcal{M})$. N^* indicates the formal adjoint of N and it is $N^* \in \text{Hom}(T_\nu^*\mathcal{M}, T_x^*\mathcal{B})$.

We cannot say many general things about the measures of deformation in the present setting because ν can have different roles with respect to them, depending on its meaning in specific theories.

In this setting, *motions* are *pairs* of time parametrized families of deformations and morphological descriptor maps

$$(x, t) \mapsto y := u(x, t) \quad \text{and} \quad (x, t) \mapsto \nu := \tilde{\nu}(x, t),$$

with t the time, ranging in some interval of the real line. For them, we assume differentiability in time, at least with piecewise differentiable first and second time derivatives. We write then

$$\dot{y} := \frac{\partial u(x, t)}{\partial t}$$

and

$$\dot{\nu} := \frac{\partial \tilde{\nu}(x, t)}{\partial t}$$

for the pertinent time rates in Lagrangian representation. \dot{y} is the macroscopic velocity, while $\dot{\nu}$ indicates the time rate of the microscopic features represented by ν . We presume also time differentiability for the first spatial derivatives of u and $\tilde{\nu}$ and write \dot{F} and \dot{N} for the pertinent rates.

5. Observers and their role

In the standard format of continuum mechanics of materials, an observer is a coordinate frame in the whole ambient space and a time scale. Changes in observers are changes of this frames. Commonly, we leave invariant the time scale or admit just affine changes in time unless we want to treat the relativistic case. In the present discussion, I consider invariant the measure of time: the observers involved have the same clock. Changes in observers in space can be isometric or not. Each possible choice determines a certain setting to be discussed because the definition of an observer in mathematical terms is essentially a way of formalizing the action of recording a mechanical phenomenon.

Requirements of invariance with respect to rigid-body-type changes in observers are commonly used to restrict possible constitutive equations through the notion of *objectivity* (an entity is objective if it changes under this type of changes in observers according to its tensor nature). However, invariance of this type can be used also to derive balance equations, as shown by Noll [35], by raising to the level of a first principle a result by Gabrio Piola.

Requirements of invariance with respect to non-necessarily rigid changes in observers allows us to prescribe what we call conditions of *covariance*, discussed extensively in [10]. We can interpret in the sense of covariance the way we compute the first variation of the energy in the (conservative) elastic case.

In any case, the space involved in the standard approaches is just the ambient point space, the physical one. There we find both the reference and the actual macroscopic configurations, although in principle endowed with different coordinate systems. In imposing objectivity, e.g., we commonly affirm that two different observers connected by a rigid-body motion evaluate the *same* reference (macroscopic) shape. Since an observer in space is a coordinate frame in the *whole* space, affirming that the reference place remains invariant under, e.g., rigid-body-type changes of frames of reference is tantamount to imagine that the reference (macroscopic) shape of the body is in a copy of the ambient space. This is the reason for the initial distinction I have made between \mathcal{E} and $\tilde{\mathcal{E}}$. So, in the end the geometric environments involved in the standard format are two,

beyond the time scale. In the setting discussed here, there is another geometric environment: the manifold \mathcal{M} of microstructural shapes. These remarks then lead to the following definition:

Definition 5.1. An *observer* is a collection of coordinate systems (*atlas*, in short) over *all* the geometrical environments necessary to describe the morphology of a body and its motion.

An axiom implicitly adopted in standard treatments is that *two different observers must perceive the same type of material*. Consequently, changes of the atlas in the reference space must be also material isomorphisms. The traditional notion introduced by Noll [8] requires to be extended to the present multifield setting but, in any case, the condition requiring the conservation of the referential mass density persists, so that changes of frames in the reference space must be volume preserving, independently of the circumstance that we analyse solids or fluids, to agree with the axiom just mentioned. Commonly, such an axiom of *permanence of the material typology* under changes in observers is not rendered explicit but it is implicitly used in the Nöther theorem, the Marsden–Hughes theorem and, above all, when we compute the horizontal variation of the elastic energy in finite-strain elasticity.

We can define different changes in observers. We list those that we consider essential for developing a unifying framework for the mechanics of complex materials and we do not consider changes in the time scale.

(a) Synchronous isometric-type changes in observers in multi-field setting

Consider smooth maps $t \mapsto a(t) \in \mathbb{R}^3$ and $t \mapsto Q(t) \in \text{SO}(3)$, with $\text{SO}(3)$ the space of orthogonal second-rank tensors on \mathbb{R}^3 with unitary positive determinant, and define a change in observer in the physical ambient space $\tilde{\mathcal{E}}^3$ by

$$y \mapsto y' := a(t) + Q(t)(y - y_0),$$

where y_0 is an arbitrary fixed point. y and y' are the places of the same material element recorded, respectively, by two observers \mathcal{O} and \mathcal{O}' . They differ from one another by the rigid-body motion just defined, characterized by translation $a(t)$ and rotation $Q(t)$. By computing the time derivative of y' and pulling back from \mathcal{O}' to \mathcal{O} the velocity y' , we define a new velocity \dot{y}^* to be

$$\dot{y}^* := Q^T \dot{y}' = c(t) + q(t) \times (y - y_0) + \dot{y}, \quad (5.1)$$

a standard relation in which $c := Q^T \dot{a}$ and q is the axial vector of the skew-symmetric tensor $Q^T \dot{Q}$.

Changing coordinates in the physical space alters also the perception of the microstructures, which are, in fact, *in* that space, within the deformed configuration, once u has been applied. Their separate representation on the manifold \mathcal{M} is just a model choice, which must account the physical perception of the body. For this reason, we define a *link* between changes in observers in the physical space, determined in general by elements of $\text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3)$, the space of one-to-one differentiable maps with differentiable inverse (*diffeomorphisms* in short) of $\tilde{\mathcal{E}}^3$ onto itself—rotations and translations are special cases—and transformations of the atlas on the manifold \mathcal{M} , given by elements of $\text{Diff}(\mathcal{M}, \mathcal{M})$, the group of diffeomorphism mapping \mathcal{M} onto itself. Formally, the link we imagine is given by a family of differentiable homomorphisms

$$\{\lambda : \text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3) \longrightarrow \text{Diff}(\mathcal{M}, \mathcal{M})\},$$

which can be even empty. We do not need to render explicit λ for constructing a general model-building framework. The specific choice of λ depends on the special cases we explore every time. When the change in observer in the physical ambient space is of rigid-body-type, as above, the set just defined reduces to

$$\{\lambda : \text{SO}(3) \longrightarrow \text{Diff}(\mathcal{M}, \mathcal{M})\}.$$

The counterpart of \dot{y}^* is given by

$$\dot{v}^* = \dot{v} + \mathcal{A}(v)q, \quad (5.2)$$

with $\mathcal{A}(v) \in \text{Hom}(\mathbb{R}^3, T_v\mathcal{M})$. When $\text{SO}(3)$ is not included in $\text{Diff}(\mathcal{M}, \mathcal{M})$ and the set $\{\lambda\}$ is not empty, by indicating by $v_{\lambda(Q)}$ the value of v after the action of $\lambda(Q) \in \text{Diff}(\mathcal{M}, \mathcal{M})$ (once again the explicit expression of $v_{\lambda(Q)}$ depends on the tensorial nature of v and $\lambda(Q)$), $\mathcal{A}(v)$ is given by

$$\mathcal{A}(v) = \left. \frac{dv_{\lambda(Q)}}{d\lambda} \frac{d\lambda(Q)}{dq} \right|_{q=0},$$

with $q(t) \in \mathbb{R}^3$ the value of a smooth map $t \mapsto q(t)$ such that $Q(t) = \exp(-\mathbf{e}q(t))$, \mathbf{e} Ricci's symbol. Otherwise, we get

$$\mathcal{A}(v) = \left. \frac{dv_q}{dq} \right|_{q=0}.$$

For example, when \mathcal{M} coincides with \mathbb{R}^3 , we find $\mathcal{A} = v \times$. The choice of the relation (5.2) points out that the microstructural descriptor is *insensitive* to rigid translations in space of the whole body. In fact, v at a point describes what is *inside* the material element placed there: it brings information about the inner structure, which translates with the point and changes independently of the translation itself.

Isometric-type changes in observers pertain also to the space where we select the reference configuration. Let w the value at x and t of a vector field over the reference space. An observer in this space is once again a coordinate frame. We indicate by w' the values of the considered vector field after rotating and translating the coordinate frame. The pull-back of w' to the first observer gives a transformation rule analogous to (5.1), a rule defining w^* , namely

$$w^* := \bar{c}(t) + \bar{q}(t) \times (x - x_0) + w, \quad (5.3)$$

where x_0 is another arbitrary fixed point, \bar{c} a translation and \bar{q} a rotation vector.

(b) Diffeomorphism-based changes in observers

- Over the ambient space, we may consider the action of a time-parametrized class of elements of $\text{Diff}(\mathcal{E}^3, \mathcal{E}^3)$. Precisely, we define smooth maps $t \mapsto h_t : \mathcal{E}^3 \rightarrow \mathcal{E}^3$, with $h_t \in \text{Diff}(\mathcal{E}^3, \mathcal{E}^3)$ and $h_0 = \text{identity}$. The smoothness of h_t in time defines a velocity field $y \mapsto \bar{v} := (d/dt)h_t|_{t=0}$ and the relation (5.1), i.e. the change $\dot{y} \rightarrow \dot{y}^*$, becomes

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

- The class of differentiable homomorphisms λ generate over \mathcal{M} maps $\lambda(h_t) : \mathcal{M} \rightarrow \mathcal{M}$. Moreover, nothing excludes in such a general setting the additional action of a time-parametrized family of elements of $\text{Diff}(\mathcal{M}, \mathcal{M})$, say $t \mapsto \tilde{h}_t : \mathcal{M} \rightarrow \mathcal{M}$, with $\tilde{h}_0 = \text{identity}$, smooth with respect to time. Let us write v for the velocity $(d/dt)\tilde{h}_t|_{t=0}$. The relation (5.2), i.e. the change $\dot{v} \rightarrow \dot{v}^*$, becomes

$$\dot{v} \rightarrow \dot{v}^\# := \dot{v} + v + \frac{1}{2}\mathcal{A}(v)\text{curl}\bar{v},$$

where $\frac{1}{2}\text{curl}\bar{v}$ is the spin of the velocity \bar{v} ; it plays the role of q in (5.2).

- Finally, over the reference space we may consider the action of a time-parametrized class of elements of $\text{Diff}(\mathcal{E}^3, \mathcal{E}^3)$. Then we define smooth maps $t \mapsto \hat{h}_t : \mathcal{E}^3 \rightarrow \mathcal{E}^3$, with $\hat{h}_t \in \text{Diff}(\mathcal{E}^3, \mathcal{E}^3)$ and $\hat{h}_0 = \text{identity}$ and write \bar{w} for the velocity $(d/dt)\hat{h}_t|_{t=0}$. The relation (5.3), i.e. the change $w \rightarrow w^*$, becomes

$$w \rightarrow w^\# := w + \bar{w}.$$

However, according to the axiom of permanence of the material typology under changes in observers mentioned above, changes in observers over the reference place should be described by maps preserving the mass, i.e. the volume. Consequently, \hat{h}_t should be selected in the special subgroup of volume-preserving diffeomorphisms.

6. Origin and nature of the balance equations

In the standard format of continuum mechanics, we distinguish into bulk and surface actions exchanged by a part of a body with the rest of the body and the environment. Such actions can be defined as functionals over the algebra of bodies constituting the universe [8,12] or by the power that they develop in the rate of change of the body's shape [7,35]. Bulk actions describe the action of the gravitational or electromagnetic fields, while the contact ones among portions of the body can be interpreted as averages of the molecular or atomic links in the material.

Intending the definition of actions in terms of the power that they develop on the rate of change of the body's shape furnishes us an immediate view on them once we have decided the way we describe the body's morphology.

Then, the problem is to establish the balance equations that they satisfy, specifically the ones involving actions determined by the microstructural changes. We list here various ways at our disposal to get balance equations in continuum models of the material behaviour. They are divided in two groups.

In the *first group*, no list of state variables comes into play.

- (1) We can assign directly *point-wise balances*.
- (2) We can assume the form of *integral balances*, deriving the point-wise counterparts by presuming that they hold for any subset of the body with non-vanishing volume and appropriate regularity (the Euler principle).
- (3) We can presume the validity of the *principle of the virtual power*, after the assumption of the structure of external and internal (or inner) powers.
- (4) We can presume the expression of the *external power* alone and require its *invariance* under rigid-body-type changes in observers.
- (5) In presence of material mutations, altering the geometry of the material structure of a body, the notion of external power requires an extension to that of *relative power*, specified below. For it, we require the invariance with respect to a class of rigid-body-type changes in observers, including the reference space.
- (6) We can get balance equations *from discrete schemes* through homogenization procedures (e.g. [36,37]). A fruitful, challenging portion of this path is the evaluation of the continuum limit of the Boltzmann equation [23].

The *second group* of possible paths involves the choice of the list of state variables, so that we put on the same conceptual level the derivation of the balance equations and the (at least preliminary) assignment of the constitutive equations.

- (7) We can evaluate, in fact, the *first variation* of some *energy*, even including dissipation potentials (in this case, we have expressions of the so-called d'Alembert–Lagrange principle).
- (8) We can impose a *balance of energy* and require its *covariance* in the case that bulk forces can be dissipative.
- (9) We can assume an appropriate version of the *Poisson brackets*, even including *dissipative brackets* (they are connected with a dissipation potential).
- (10) We can decide a version of the *second law of thermodynamics* (even including the relative power) and require its *covariance*.

The choice of a way to act is not just a matter of taste. Different assumptions are implied. Our tendency should be to reduce them to the need of having a control as strong as possible of the theoretical structures that we use, above all when we need to extend the framework that we know to tackle the description of unusual or yet unexplored physical circumstances.

- Prescribing point-wise balances of the actions occurring in complex materials in analogy with the standard instances is a direct jump to the end of the discussion about balance

equations. When we act in this way, beyond the structure of the equations, we presume the representation of the microstructural contact actions in terms of microstresses and self-actions, without having proven the analogous of Cauchy's theorem for the standard tension. In its original formulation, such a theorem requires the boundedness of the bulk actions, the knowledge of the integral balance of forces, and the action–reaction principle. If we choose to act in this way, we have to remind that we are not sure about the effectiveness of the result: analogy, in fact, is not always a secure path.

- The direct assignment of integral balances demands fewer assumptions, in fact, and allows to try to prove Cauchy-type theorems. However, since we consider \mathcal{M} as a nonlinear manifold, which is the general unifying choice, prescribing an independent integral balance of micro-actions would be highly questionable formally. We would write, in fact, integrals involving integrands taking values on the cotangent bundle of \mathcal{M} , which is a nonlinear space (unless \mathcal{M} coincides with a linear space) and is the target space of the integrand, so the definition of the integral itself would be questionable. Moreover, if we consider \mathcal{M} to be coincident with a linear space, we can see that such a balance would be essentially superfluous, as shown in a theorem below.
- When we adopt the principle of virtual power (as in [38]), we are directly *prescribing* the *weak form* of the point-wise balance equations, the form used in computational procedures. The choice implies also the presumption of the expression of the contact actions in terms of stress. The proof of a Cauchy-type theorem would require the use of the integral balances, rendering superfluous the virtual power principle. In other words, in the principle of virtual power we presume *a priori* all the ingredients appearing in the balance equations, without proving the existence of the standard and microstructural stresses and the possible self-actions. There is also a subtle connection between integral balances and the principle of virtual power, or virtual work, depending on whether we use the velocity or the displacement, the one shown in [39].
- The procedure based on the invariance of the power of external actions over a generic part of a body in a continuum representation is the one demanding the fewest assumptions and can be used when the reference place is fixed once and for all. I present here some details of it, with appropriate references, because in the multi-field setting discussed here, it is a tool for deriving clearly balance equations in both integral and point-wise form.
- The idea of the relative power is an extension of the previous procedure when macroscopic structural changes in the body suggest the adoption of multiple reference shapes. It allows us to derive from a unique source not only the action–reaction principles for standard and microstructural actions (an unusual form in the latter case), the expressions of the contact actions in terms of stress and the balance equations, but also the balances of configurational actions from a unique source. Pertinent details also appear below.
- Rigid-body-type changes in observers pertain to the first set in the list above of sources of balance equations. The second set involves non-rigid changes in observers so that the word *covariance* appears repeatedly. Its typical occurrence is in Nöther's theorem, based on the requirement of *invariance* of the Lagrangian density with respect to the action of families of diffeomorphisms on both spatial and referential coordinates. In the last case, the one involving the referential shape, the diffeomorphisms considered must be volume preserving if we want that two different observers perceive the *same type* of material, as already recalled, irrespectively of whether we are thinking of solids or fluids. Classes of changes in observers and those of admissible motions are not necessarily coincident, in fact, as it is well known from elementary courses.
- Besides the Lagrangian format in the conservative setting, we can describe motions in terms of the Hamiltonian, either through the Hamilton equations or to their weak form represented by the Poisson brackets, which can be supplemented by appropriate dissipative brackets where there are effects that can be associated with a dissipation potential (e.g. [40,41]), as a sort of counterpart of the d'Alembert–Lagrange principle.

- In the presence of dissipative bulk external actions, not necessarily associated with a dissipation potential, covariance appears in Marsden–Hughes’s theorem [10]. In its original version, the theorem refers to finite-strain elastodynamics of simple bodies. What is required is the covariance—intended as structural invariance of the principle with respect to diffeomorphisms acting on the ambient space—of the first principle of thermodynamics in isothermal conditions: the balance of mechanical energy. The result is the representation of the standard tension in terms of the stress tensor (i.e. Cauchy’s theorem), the point-wise balances, the *a priori* constitutive restrictions on the stress. We can generalize it to the multi-field setting treated here, even writing the first principle in terms of relative power.
- Marsden–Hughes’s theorem is a variation of the Nöther’s theorem towards the presence of dissipative structures. What should we imagine for phenomena involving irreversible strain (as in plasticity) or dissipative stress components (as in viscoelasticity)? For finite-strain plasticity, a theorem proven in 2013 furnishes the answer [42]. Versions of it apt for traditional viscoelasticity and the multi-field setting for complex materials are possible.

(a) The procedure based on the invariance of the external power under isometric-type changes in observers

Details on the procedure based on the invariance of the external power over a generic part of a body viewed at continuum scale help in clarifying the previous remarks.

Let us call a *part* of the body in its reference place any subset of \mathcal{B} with non-vanishing volume and the same (geometric) regularity of \mathcal{B} itself.

We define the *power of external actions on a generic part of \mathcal{B}* (external power in short) as the functional $\mathcal{P}_b^{\text{ext}}$, linear on the rates \dot{y} and \dot{v} and additive over disjoint parts, defined by

$$\mathcal{P}_b^{\text{ext}}(\dot{y}, \dot{v}) := \int_b (b^\dagger \cdot \dot{y} + \beta^\dagger \cdot \dot{v}) dx + \int_{\partial b} (t \cdot \dot{y} + \tau \cdot \dot{v}) d\mathcal{H}^2,$$

where $b^\dagger(x) \in T_{u(x)}^* \mathcal{B}_a$ represents body forces (the sum of inertial and non-inertial components) and $t(x) \in T_{u(x)}^* \mathcal{B}_a$ is the traction through the boundary of b ; $\tau(x) \in T_{\dot{v}(x)}^* \mathcal{M}$ indicates microstructural contact actions, while $\beta^\dagger(x) \in T_{\dot{v}(x)}^* \mathcal{M}$ their external bulk counterparts over the microstructure alone. $d\mathcal{H}^2$ is the ‘surface’ measure over ∂b . The dot between two generic symbols denotes the duality pairing both in the expression of $\mathcal{P}_b^{\text{ext}}(\dot{y}, \dot{v})$ and in any occurrence below.

By assumption both t and τ depend on x and n at every instant t . In other words, Cauchy’s assumption about the dependence on the standard traction on the normal to the boundary of the part considered is extended to the microstructural contact actions.

When we write such an expression of the power, we presume that the reference shape is fixed once and for all. We then subordinate $\mathcal{P}_b^{\text{ext}}$ to an axiom of invariance.

Axiom of power invariance in a complex material [43]: *The external power on a generic part b or the whole B is invariant under isometry-based changes in observers, i.e.*

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

for any choice of c and q , and the part considered.

The axiom has stringent consequences.

Theorem 6.1. [43,44] *The invariance of the external power under isometric-type changes in observers implies the following statements:*

(1) *The integral balances*

$$\int_b b^\dagger dx + \int_{\partial b} t d\mathcal{H}^2 = 0, \quad (6.1a)$$

$$\int_b ((y - y_0) \times b^\dagger + \mathcal{A}^* \beta^\dagger) dx + \int_{\partial b} ((y - y_0) \times t + \mathcal{A}^* \tau) d\mathcal{H}^2 = 0, \quad (6.2)$$

where \mathcal{A}^* is the formal adjoint of \mathcal{A} , i.e. $\mathcal{A}^*(v) \in \text{Hom}(T_v\mathcal{M}, \mathbb{R}^3)$, hold.

- (2) The standard traction (here expressed in Lagrangian representation) satisfies the action–reaction principle:

$$\mathfrak{t}(x, n) = -\mathfrak{t}(x, -n). \quad (6.3)$$

- (3) The microstructural contact actions satisfy a non-standard action–reaction principle:

$$\mathcal{A}^*(\tau(x, n) + \tau(x, -n)) = 0. \quad (6.4)$$

- (4) If $|b^\ddagger|$ is bounded over \mathcal{B} and $\mathfrak{t}(\cdot, n)$ is a continuous function of x , $\mathfrak{t}(x, \cdot)$, a function of n , is homogeneous and additive, i.e. there exists a second-rank tensor field $x \mapsto P(x)$ such that

$$\mathfrak{t}(x, n) = P(x)n(x), \quad (6.5)$$

where

$$P(x) = \sum_{K=1}^3 \mathfrak{t}(x, e_K) \otimes e_K \in \text{Hom}(T_x^*\mathcal{B}, T_{u(x)}^*u(\mathcal{B}))$$

is the first Piola–Kirchhoff stress and e_K is the k th vector of a basis in a neighbourhood of x (Cauchy’s theorem in referential form).

- (5) If in addition to the previous assumptions $|\mathcal{A}^*\beta^\ddagger|$ is bounded over \mathcal{B} and $\tau(\cdot, n)$ is a continuous function of x , $\tau(x, \cdot)$, as a function of n , is homogeneous and additive, i.e. there exists a second-rank tensor field $x \mapsto S(x)$ such that

$$\tau(x, n) = S(x)n(x),$$

where

$$S(x) = \sum_{K=1}^3 \tau(x, e_K) \otimes e_K \in \text{Hom}(T_x^*\mathcal{B}, T_v^*\mathcal{M})$$

is the so-called microstress.

- (6) If the fields $x \mapsto P$ and $x \mapsto S$ are in $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$ and the fields $x \mapsto b$, $x \mapsto \beta^\ddagger$ are continuous over \mathcal{B} , the point-wise balance of forces

$$\text{Div}P + b^\ddagger = 0 \quad (6.6)$$

holds and there exists a field $x \mapsto z(x) \in T_v^*\mathcal{M}$ such that

$$\text{Div}S + \beta^\ddagger - z = 0 \quad (6.7)$$

and

$$\text{Skw}PF^* = \frac{1}{2}e(\mathcal{A}^*z + (D\mathcal{A}^*)S). \quad (6.8)$$

- (7) The equation

$$\mathcal{P}_b^{\text{ext}}(\dot{y}, \dot{v}) = \int_b (P \cdot \dot{F} + z \cdot \dot{v} + S \cdot \dot{N}) dx \quad (6.9)$$

holds and we call internal (or inner) power the right-hand side term.

Proof. The first item follows trivially by the arbitrariness of c and q because the axiom implies

$$\mathcal{P}_b^{\text{ext}}(c + q \times (y - y_0), \mathcal{A}q) = 0$$

The first integral balance (6.1a) implies the boundedness of the absolute value of the traction average over the boundary of any part, once the bulk actions are bounded. Consequently, standard arguments [12] allow us to obtain the action–reaction principle (6.3) for \mathfrak{t} and the Cauchy theorem (6.5) about the existence of a stress independent of n . Note that the existence of the stress tensor can be obtained in less stringent regularity assumptions (e.g. [45,46]).

On defining $r := (y - y_0) \times b^\ddagger + \mathcal{A}^* \beta^\ddagger$ and $p := (y - y_0) \times \mathfrak{t} + \nu \times \tau$, the integral equation (6.2) writes obviously as

$$\int_{\mathfrak{b}} r \, dx + \int_{\partial \mathfrak{b}} p \, d\mathcal{H}^2 = 0.$$

Since y_0 is arbitrary, once we choose y , we can select y_0 such that the above boundedness assumption about $|b^\ddagger|$ over \mathcal{B} may imply the one of $(y - y_0) \times b^\ddagger$. Moreover, the above assumption of the boundedness $|\mathcal{A}^* \beta^\ddagger|$ over \mathcal{B} implies the one of r . The assumed boundedness of the first integral implies the one of the absolute value of the right-hand side term, so that we can apply the standard procedure adopted for the traction \mathfrak{t} [12], obtaining a non-standard action–reaction principle (6.4). We find, in fact,

$$p(x, n) = -p(x, -n),$$

i.e.

$$(y - y_0) \times (\mathfrak{t}(x, n) - \mathfrak{t}(x, -n)) + \mathcal{A}^*(\tau(x, n) - \tau(x, -n)) = 0,$$

so that from (6.3) we find (6.4).

Not writing explicitly time for the sake of conciseness, we can use a tetrahedron type argument to show the linearity of p with respect to n , namely we show the existence of a second-rank tensor $A(x)$ such that

$$p(x, n) = A(x)n(x).$$

Then we find

$$(y(x) - y_0) \times \mathfrak{t} + \mathcal{A}^* \tau = (y(x) - y_0) \times P(x)n(x) + \mathcal{A}^* \tau = A(x)n(x),$$

so that

$$\mathcal{A}^* \tau(x, n) = A(x)n(x) - (y(x) - y_0) \times P(x)n(x),$$

which implies the linearity of $\tau(x, n)$ with respect to n because \mathcal{A}^* does not depend on n .

The localization of the integral balance of forces, namely equation (6.1a), which is possible due to the arbitrariness of \mathfrak{b} , gives rise to the local balance (6.6). By contrast, the localization of the integral balance (6.2) implies

$$\mathcal{A}^*(\text{Div} S + \beta^\ddagger) = eP^* - (D\nu)^* S,$$

which indicates the existence of a covector, say z , satisfying equation (6.7) with constraint (6.8). The last item follows by using the pointwise balances and Gauss's theorem. ■

- z is a local action, the one of the microstructure ‘inside’ the material element at x over itself. S measures the first-neighbour interactions due to inhomogeneous microstructural changes among neighbouring material elements.
- If we would start from the last relation in the theorem as a first principle—it would correspond to a principle of virtual power, when we allow the rates to be virtual—it would impose the existence of the self-action and the stresses, in other words, we would presume *a priori* the structure of the balance equations.
- The theorem indicates also that the assumption *a priori* of the existence of an independent *integral* balance of microstructural actions can be considered superfluous. The circumstance that such actions appear in the (generalized) balance of torques does not imply at all that they are couples for the presence of the linear operator \mathcal{A}^* . *Per se* the microstructural actions are not necessarily couples, while their projection through \mathcal{A}^* into the ambient physical space generates couples.
- Non-trivial questions pertain to *boundary conditions* to be prescribed for the balance of microstructural actions. Formally, they can be of Dirichlet or Neumann type. The field $\bar{\nu}$ can be assigned experimentally along $\partial \mathcal{B}$ in some specific circumstances, as it is for liquid crystals for which surfactants can impose the orientation of the molecules at the boundary. As regards the prescription of micro-tractions $\tau = Sn$ along $\partial \mathcal{B}$, unless we know a loading device able to prescribe direct contact actions over the microstructure, we

have to impose simply $\mathcal{S}n = 0$. A case $\mathcal{S}n \neq 0$ occurs when we use the present framework to construct direct models of rods and shells so that we may prescribe, e.g., external bending moments at the boundary [47].

- As regards *inertia effects*, we may presume that the bulk actions can be decomposed *additively* into inertial and non-inertial contributions, the former indicated by a superscript ‘in’:

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

By raising at a first principle a version of the so-called *theorem of live loads*, we can presume that the inertial components of the bulk actions can be identified by imposing that their power equals the negative of the rate of the kinetic energy, and we write

$$\frac{d}{dt} \int_b k(\dot{y}^b, v, \dot{v}^b) dx + \int_b (b^{\text{in}} \cdot \dot{y} + \beta^{\text{in}} \cdot \dot{v}) dx = 0, \quad (6.10)$$

where $k(\dot{y}^b, v, \dot{v}^b)$ is the *kinetic energy*, \dot{y}^b is defined by $\dot{y}^b := \tilde{g}j\dot{y}$, and \dot{v}^b is in $T_v^* \mathcal{M}$. We consider [32] the possible presence of microscopic (relative) inertia. Cases in which it may occur are, for example, those of bubbles migrating inside a liquid in motion, relatively to it, and vibrating within it [48], or solids with an enormous number of cavities, each one containing a gyroscope [49,50]. In accordance to a proposal by Capriz [32], we write the decomposition

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

where ρ is the referential mass density and κ is such that $\kappa(v, 0) = 0$; it admits non-negative definite second derivative with respect to \dot{v}^b , i.e. $\partial \kappa(v, \dot{v}^b) / \partial \dot{v}^b \partial \dot{v}^b \cdot (\dot{v}^b \otimes \dot{v}^b) \geq 0$, the equality sign holding when $\dot{v}^b = 0$. The dependence of $\kappa(v, \dot{v}^b)$ must be considered deprived by the effects of macroscopic rigid-body motion so that we may consider κ as a function

$$\kappa(v, \dot{v}^b) = \mathfrak{h}(v, \dot{v}^b - (Aq)^b).$$

The choice prevents an incongruence which would occur, by contrast, when κ is quadratic with respect to \dot{v}^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} . By inserting the previous assumptions in the integral balance (6.10), the arbitrariness of the part considered implies the identifications $b^{\text{in}} = -\rho \dot{y}$ and $\beta^{\text{in}} = (d/dt) \partial \chi(v, \dot{v}) / \partial \dot{v} - \partial \chi(v, \dot{v}) / \partial v$, with $\chi : T\mathcal{M} \rightarrow \mathbb{R}^+$ a C^1 function such that $\kappa(v, \dot{v}^b) := \partial \chi(v, \dot{v}) / \partial \dot{v} \cdot \dot{v} - \chi(v, \dot{v})$, at any \dot{v} , with $\dot{v}^b := \partial \chi(v, \dot{v}) / \partial \dot{v}$.

(b) The relative power and its invariance

Let us relax the idea that the reference place is fixed once and for all. This choice becomes physically weighty when we consider structural irreversible changes in the material structure, which frustrate even partially the one-to-one correspondence between the reference shape and the actual one at each instant. Examples are nucleation and/or evolution relative to the rest of the body of fractures or bulk inhomogeneities along a motion. At a given instant the actual shape of a body is not in one-to-one correspondence with the initially chosen reference shape but with a copy of it differing by the (virtual) pre-image of the defect.

A way of describing such circumstances is to make use of *multiple reference shapes*. However, instead of considering a family of infinitely many possible reference shapes for the body under scrutiny, it suffices to introduce a sort of *infinitesimal generator* of the family itself: a (not necessarily integrable) vector field

$$x \mapsto w := \tilde{w}(x) \in \mathbb{R}^3$$

over the reference shape. Then we define a power relative to the virtual rate w . The definition considers three key aspects: (i) the velocities \dot{y} and w are not in the same space so we have to push forward w in the ambient space or to pull back \dot{y} into the reference space to compare them; (ii)

an effect of the mutation is the rupture and reformation of the material bonds so that we may include configurational forces and couples, the latter ones determined also by possible changes in the material symmetry and (iii) a mutation alters the energetic landscape.

We consider the following ingredients:

- (a) the *free energy* ψ that we presume to be a differentiable function of x, t and a list ζ of state variables that we leave here *undetermined*—no constitutive equations enter into play—and
- (b) bulk configurational forces f with dissipative nature and couples μ , which have, in contrast, both dissipative and conservative components.

We then define *relative power* [44] the functional $\mathcal{P}_b^{\text{rel}}$ given by

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

with

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

and

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

Above, $\partial_x \psi$ is the *explicit derivative* of $\psi = \tilde{\psi}(x, t, \zeta)$ with respect to x , holding fixed ζ . It accounts for the inhomogeneity in the energy landscape, altered by the mutation. The term $(n \cdot w) \psi$ is the flux energy density across the boundary ∂b , due to the mutation itself.

As for the external power, we subordinate $\mathcal{P}_b^{\text{rel}}$ to an axiom of invariance.

Axiom of invariance for the relative power [44]: *The relative power is invariant under isometry-based changes in observers, i.e.*

$$\mathcal{P}_b^{\text{rel}}(\dot{y}, \dot{v}, w) = \mathcal{P}_b^{\text{rel}}(\dot{y}^*, \dot{v}^*, w^*)$$

for any choice of c, q, \bar{c}, \bar{q} and any part b

Even in this case we have stringent consequences.

Theorem 6.2. *The assumed invariance of the relative power under isometric-type changes in observers implies the validity of the results 1 to 6 in theorem 6.1 and the following additional statements:*

- (i) *The integral configurational balances*

$$\begin{aligned} & \int_{\partial b} \mathbb{P}n \, d\mathcal{H}^2 - \int_b (F^* b^\dagger + N^* \beta^\dagger) \, dx - \int_b (\partial_x \psi + f) \, dx = 0, \\ & \int_{\partial b} (x - x_0) \times \mathbb{P}n \, d\mathcal{H}^2 - \int_b (x - x_0) \times (F^* b^\dagger + N^* \beta^\dagger) \, dx \\ & - \int_b (x - x_0) \times (\partial_x \psi + f) \, dx + \int_b 2\mu \, dx = 0, \end{aligned}$$

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

- (ii) *If the field $x \mapsto \mathbb{P}$ is in $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$ and $x \mapsto F^* b, x \mapsto f, x \mapsto \partial_x \psi$ are continuous over \mathcal{B} , the pointwise configurational balances*

$$\begin{aligned} \text{Div} \mathbb{P} - F^* b^\dagger - N^* \beta^\dagger + \partial_x \psi &= f, \\ \text{Skw}(g^{-1} \mathbb{P}) &= -2\bar{e}\mu, \end{aligned}$$

with \bar{e} Ricci's symbol with all contravariant components, namely \bar{e}^{ABC} , hold.

(iii) *The equation*

$$\mathcal{P}_b^{\text{rel}}(\dot{y}, \dot{v}, w) = \int_b (P \cdot \dot{F} + z \cdot \dot{v} + S \cdot \dot{N} + \mathbb{P} \cdot Dw + \mu \cdot \text{curl} w) dx$$

holds and we call extended internal (or inner) power the right-hand side term.

The balance equations above have to be accompanied by the choice of the constitutive structures, which specify the material class and are closure conditions for the system of equations. The Clausius–Duhem inequality helps in limiting a priori constitutive structures. Here we write it in isothermal version as

$$\dot{\Psi}(b) - \mathcal{P}_b^{\text{ext}}(\dot{y}, \dot{v}) \leq 0,$$

and we presume it to hold for any choice of the rates involved and any part b , with $\dot{\Psi}$ the time rate of the total free energy of b . By using equation (6.9) and considering $\Psi(b)$ as given by $\int_B \psi dx$, when the free energy density ψ , the stresses P , S and the self-action z depend all on x, F, v, N only, the inequality imposes $P := \partial\psi/\partial F$, $z := \partial\psi/\partial v$, $S := \partial\psi/\partial N$. When it is the case, dissipative components of P , S and z are considered to be additive to the ‘energetic’ parts, always determined by the first derivatives of the free energy density with respect to its entries.

(c) The conservative setting: Hamiltonian structures

When we put on the same level the representation of the actions and the prescription of the constitutive structures, to get balance equations we may resort to one of the paths indicated in the second group of possibilities above listed. In particular, when we restrict our attention to elastic complex bodies, a Lagrangian density \mathcal{L} exists, so that the total Lagrangian L_B is given by

$$L_B = \int_B \mathcal{L}(x, y, \dot{y}, F, v, \dot{v}, N) dx,$$

where we presume that \mathcal{L} be of the form

$$\mathcal{L}(x, y, \dot{y}, F, v, \dot{v}, N) = \frac{1}{2} \rho \dot{y}^b \cdot \dot{y} + \chi(v, \dot{v}) - e(x, F, v, N) - \mathfrak{w}(y, v),$$

with e the elastic energy density and \mathfrak{w} the density of the potential of external actions. Then we find balances of forces and micro-actions on the basis of Hamilton’s principle, by computing the first variation of L_B with respect to the action of diffeomorphisms over \mathcal{E} and \mathcal{M} (the so-called *vertical variation*), and equating the results to zero. The resulting equations are

$$\overline{\frac{\partial \mathcal{L}}{\partial \dot{y}}} = \frac{\partial \mathcal{L}}{\partial y} - \text{Div} \frac{\partial \mathcal{L}}{\partial F} \quad (6.11)$$

and

$$\overline{\frac{\partial \mathcal{L}}{\partial \dot{v}}} = \frac{\partial \mathcal{L}}{\partial v} - \text{Div} \frac{\partial \mathcal{L}}{\partial N}. \quad (6.12)$$

— When we presume the existence of an internal constraint of the type

$$v = f(F),$$

with f a differentiable function, we recover *strain-gradient elasticity* as a special case of the general format of the elasticity of complex materials, as shown in [51]. In this case, the microstress becomes the third-rank hyperstress appearing in the direct formulation of strain-gradient elasticity (the proof of the existence of \mathcal{S} indicated above applies).

— The pair (v, N) is the peculiar element of the tangent map $T\bar{v}(x): T_x \mathcal{B} \rightarrow T_v \mathcal{M}$. v and N cannot be separated invariantly unless \mathcal{M} is endowed with a parallel transport (and one wants also to have a physically significant parallelism). A similar remark holds also for the generic element (v, \dot{v}) of $T\mathcal{M}$. This is the basic reason allowing the presence of v in the

list of entries of e , a presence which implies also the one of the self-action z , at least in its energetic (conservative) component.

We can do something more.

Define ρ and τ , respectively, the *canonical momentum* and the *canonical microstructural momentum*, by

$$\rho = \frac{\partial \mathcal{L}}{\partial \dot{y}} \quad \text{and} \quad \tau = \frac{\partial \mathcal{L}}{\partial \dot{v}}.$$

With the previous notations we may then define what we call the *Hamiltonian density* \mathcal{H} by

$$\mathcal{H}(x, y, \rho, F, v, \tau, N) = \rho \cdot \dot{y} + \tau \cdot \dot{v} - \mathcal{L}(x, y, \dot{y}, F, v, \dot{v}, N).$$

\mathcal{H} has partial derivatives with respect to its entries; some of them are the opposite of the corresponding derivatives of \mathcal{L} so that (6.11) and (6.12) can be also written in Hamiltonian form, respectively, as

$$\left. \begin{aligned} \dot{\rho} &= -\frac{\partial \mathcal{H}}{\partial y} + \text{Div} \frac{\partial \mathcal{H}}{\partial F}, \\ \dot{y} &= \frac{\partial \mathcal{H}}{\partial \rho}; \end{aligned} \right\} \quad (6.13)$$

$$\left. \begin{aligned} \dot{\tau} &= -\frac{\partial \mathcal{H}}{\partial v} + \text{Div} \frac{\partial \mathcal{H}}{\partial N}, \\ \dot{v} &= \frac{\partial \mathcal{H}}{\partial \tau}. \end{aligned} \right\} \quad (6.14)$$

Let us consider for equations (6.13) and (6.14) boundary conditions of the type

$$u(x) = \bar{u} \quad \text{on } \partial \mathcal{B}$$

and

$$\tilde{v}(x) = \bar{v} \quad \text{on } \partial \mathcal{B}.$$

The Hamiltonian for the whole body is given by

$$H(y, \rho, v, \tau) := \int_{\mathcal{B}} \mathcal{H}(x, y, \rho, F, v, \tau, N) \, dx.$$

Consider now functionals $K(y, \rho, v, \tau)$ defined by

$$K(y, \rho, v, \tau) := \int_{\mathcal{B}} \mathcal{K}(x, y, \rho, v, \tau) \, dx,$$

with \mathcal{K} a sufficiently smooth scalar density. Define now the variational derivatives

$$\frac{\delta \mathcal{H}}{\delta y} := \frac{\partial \mathcal{H}}{\partial y} - \text{Div} \frac{\partial \mathcal{H}}{\partial F},$$

$$\frac{\delta \mathcal{H}}{\delta v} := \frac{\partial \mathcal{H}}{\partial v} - \text{Div} \frac{\partial \mathcal{H}}{\partial N},$$

$$\frac{\delta \mathcal{H}}{\delta \rho} := \frac{\partial \mathcal{H}}{\partial \rho}$$

and

$$\frac{\delta \mathcal{H}}{\delta \tau} := \frac{\partial \mathcal{H}}{\partial \tau},$$

where the variational (partial) derivatives $\delta \mathcal{H} / \delta y$ and $\delta \mathcal{H} / \delta v$ are meant to be computed by fixing ρ and allowing y to vary and holding τ , while leaving v free to vary. In this last case, the implicit assumption is that at every v we can find a copy of τ in $T_v^* \mathcal{B}$.

Then we can define (see also [47]) the *canonical Poisson bracket* $\{K, H\}$ as

$$\begin{aligned} \{K, H\} &= \int_{\mathcal{B}} \left(\frac{\delta \mathcal{K}}{\delta y} \cdot \frac{\delta \mathcal{H}}{\delta p} - \frac{\delta \mathcal{H}}{\delta y} \cdot \frac{\delta \mathcal{K}}{\delta p} \right) dx \\ &\quad + \int_{\mathcal{B}} \left(\frac{\delta \mathcal{K}}{\delta v} \cdot \frac{\delta \mathcal{H}}{\delta \tau} - \frac{\delta \mathcal{H}}{\delta v} \cdot \frac{\delta \mathcal{K}}{\delta \tau} \right) dx \end{aligned}$$

and the functional time derivative \dot{K} as

$$\dot{K} = \int_{\mathcal{B}} \left(\frac{\delta \mathcal{K}}{\delta y} \cdot \dot{y} + \frac{\delta \mathcal{K}}{\delta p} \cdot \dot{p} \right) dx.$$

Theorem 6.3. *The validity of the equation*

$$\dot{K} = \{K, H\}$$

for any K satisfying the conditions above implies the validity of the balance equations.

In the presence of dissipative effects, which can be associated with a Rayleigh-type dissipation potential, we change the equations in the above theorem with the addition of a dissipative bracket. Specifically, we write

$$\dot{K} = \{K, H\} + \{K, R\}_D, \quad (6.15)$$

with R the already mentioned dissipation and the functional $\{\cdot, \cdot\}_D$ satisfying the following assumptions:

- $\{\cdot, \cdot\}_D$ is symmetric.
- $\{R, R\}_D \geq 0$.

With R of the type

$$R := \int_{\mathcal{B}} \mathcal{R}(\tau) dx,$$

$\{\cdot, \cdot\}_D$ is defined by

$$\{K, R\}_D := \int_{\mathcal{B}} \frac{\partial \mathcal{K}}{\partial \tau} \cdot \frac{\partial \mathcal{R}}{\partial \tau} dx.$$

We can even choose equation (6.15) as a first principle, although we restrict ourselves in this case to describe dissipation structures just in terms of R .

7. Covariance of the second law

As we have already recalled, in continuum mechanics of materials the second law is commonly considered as a tool for deducing restrictions on the possible constitutive laws and a criterion of stability. In this vein, the second law is exploited in different manners (see, e.g., the critical analysis in [52]).

We can use it also as a source of the results contained in the theorems above *and* the restrictions to the constitutive relations. Here I sketch just the essential steps of the procedure. Applications to finite-strain plasticity based on the multiplicative decomposition of the deformation gradient can be found in [42].

(a) Covariance principle in dissipative setting

Let $B \leq 0$ be in short an expression of the second law for a given observer \mathcal{O} . Another observer, \mathcal{O}' , evaluate an inequality of the type $B' \leq 0$. By assumption, the link between \mathcal{O} and \mathcal{O}' is given by diffeomorphisms as described above.

In general, B' does not coincide with B . When we pull back the inequality evaluated by \mathcal{O}' into the frame(s) defining \mathcal{O} or, by contrast, we push forward B into \mathcal{O}' , by using the diffeomorphisms relating the two observers, we, respectively, get inequalities of the type $B + B^\dagger \leq 0$ or $B + B^\ddagger \leq 0$. A

question is whether and in what sense we can characterize *a priori* in some way the terms B^\dagger and B^\ddagger . The following *principle* suggests an answer.

Covariance principle in dissipative setting: *In any diffeomorphism-based change in observer, when we project the mechanical dissipation inequality evaluated by an observer into the frame defining the other, the additional term arising along the process is always non-positive.*

In other words, with such a principle we affirm that when a process is dissipative for a given observer it is so for *any* other observer.

(b) The mechanical dissipation inequality

A key point is the explicit expression of the inequality $B \leq 0$. What I suggest here is restricted to the isothermal setting and is an extended expression of the mechanical dissipation inequality. It reads

$$B(\dot{y}, \dot{v}, w; \psi, \mathbf{b}) := \frac{d}{dt} \int_{\mathbf{b}} \psi \, dx - \mathcal{P}_\mathbf{b}^{\text{rel}}(\dot{y}, \dot{v}, w) \leq 0. \quad (7.1)$$

The procedure to evaluate its covariance, i.e. its structure invariance under diffeomorphism-based changes in observers, follows the steps below.

- Select the list of state variables appearing as entries of the energy (so far they have been left unspecified in the expression of the relative power). Restrict them by the help of objectivity assumptions (see [10–14] for the pertinent techniques). In particular, besides the presence of the spatial and material metrics, in the list of state variables the metric on \mathcal{M} may appear when we consider \mathcal{M} endowed with a metric structure as in the case it is Riemannian.
- Assume *covariance* (tensoriality) of the free energy. Formally, it means that we impose at every instant t the identity

$$\psi = \psi \circ (\hat{h}_t \times h_t \times (\lambda(h_t) \times \tilde{h}_t)),$$

where the symbol \circ indicates as above standard map composition and $(\hat{h}_t \times h_t \times (\lambda(h_t) \times \tilde{h}_t))$ summarizes the combined action of \hat{h}_t , h_t , $(\lambda(h_t), \tilde{h}_t)$, those of diffeomorphism-based changes in observers over reference and ambient spaces, and the manifold \mathcal{M} of microstructural shapes, respectively. In particular, it is convenient to express in terms of time derivative of ψ the covariance condition. To this aim, we can adapt to the setting discussed here the pertinent expression introduced in the special case of finite-strain plasticity discussed in [42]. (Incidentally, as regards plasticity, should we identify v with the slip rate in single crystals or the plastic factor in the multiplicative decomposition of F , or else a function of elastic invariants, we could recover existing models of strain-gradient plasticity as special prominent offspring of the model-building framework discussed here.)

- Impose the covariance principle in dissipative setting to the mechanical dissipation inequality (7.1), written in terms of relative power.

The results that we find are

- (1) the existence of the stress and the microstress, the latter one obtained without embedding the manifold of microstructural shapes into a linear space;
- (2) the need of a bulk inner microstructural self-action to assure local balances;
- (3) point-wise balances of standard, microstructural and configurational balance equations and
- (4) *a priori* constitutive restrictions.

They all emerge from a unique invariance requirement.

Note that, in general, under diffeomorphism-based changes of frames, as described above, since ψ is a density with respect to the volume measure, we should have

$$\psi = \det(D\hat{h}_t)\psi \circ (\hat{h}_t \times h_t \times (\lambda(h_t) \times \tilde{h}_t)).$$

The assumed covariance implies

$$\det(D\hat{h}_t) = 1,$$

i.e. that \hat{h}_t must be volume preserving, *independently of the material nature of the body*. Such a restriction on the changes in observers, that is exactly the one adopted in computing the horizontal variation of functionals in calculus of variations (see the treatise [53], where the independence between balance of forces and the one of configurational action is pointed out), agrees also with the axiom of permanence of the material typology under changes in observers.

8. Some open problems

In a 2002 lucid paper [16], John M. Ball indicated a number of open mathematical problems in nonlinear elasticity of simple bodies in the scenario opened by basic existence results in the matter [15,54,55]. A question is in what sense that problems can be discussed in the setting sketched here when we focus attention on nonlinear elasticity of complex (rather than simple) bodies. General existence results of minimizers of energy for nonlinear elastic complex materials exist. One of them is in reference [56]; its proof requires the embedding of the manifold \mathcal{M} into a linear space. The embedding is always possible because \mathcal{M} is taken to be finite-dimensional but it is not unique and we can prove existence for any embedding. A previous result is in reference [57] and deals with the micromorphic case in which \mathcal{M} is identified with a linear space. The coercivity assumption is weaker than the one adopted in [56]. However, the energy considered in reference [57] has just a decomposed structure (it is less general than the energy analysed in [56]), which allows the weaker coercivity assumption. Moreover, the use of currents in reference [56] allows us to get results in Sobolev spaces $W^{1,p}$, with p lesser than 2 and even as close as you want to 1. A general existence result avoiding embedding \mathcal{M} in any linear space, but taking \mathcal{M} as a complete Riemannian manifold and considering *multi-valued* microstructural descriptor maps (values defined to within a permutation), included in Ginzburg–Landau-type energies, appears in [58].

Discussing the possible counterparts (if any) in this setting of the problems indicated in [16] would require a paper a part. However, at least a problem can be indicated here: (*Problem 1*) What kind of regularity results can we get in nonlinear elasticity of complex bodies, i.e. with reference to energies of the type

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

with density e assumed to be polyconvex in F and convex in N , or polyconvex in the pair (F, N) , leaving \mathcal{M} not embedded but requiring that it is Riemannian?

Besides statics, dynamics indicates also unexplored lands. There are existence results in special cases of the dynamics of complex materials (e.g. [59]), but a basic question is the following: (*Problem 2*) What can we say about existence and regularity of solutions to the balance equations in Theorem 1 when we consider inertia as indicated in commenting the theorem, and what about the qualitative behaviour of trajectories?

Macroscopic inertia can be coupled with *diffusion* of the microstructures, so that the balance equation (6.7) can have parabolic nature, due to absence of microscopic inertia but presence of a dissipative self-action z , which is then proportional to the time rate of ν . (*Problem 3*) What can we say about existence in this general case, with the restrictions above?

In selecting \mathcal{M} , we implicitly imagine to have a determinate view on the microstructural features that we consider prominent. In a certain sense, we are presuming a certain uniformity in the typology of microstructures throughout the body. A closer look to physical cases can evidence circumstances of high heterogeneity, which could suggest us to consider the field

\bar{v} as stochastic. (*Problem 4*) What can we say for the general structure sketched above in this case?

Besides analytical and geometrical problems, the modelling questions are manifold. I indicate just a couple of them in the general framework, to make some examples of possibilities, leaving understood that if we look at special cases they multiply.

A problem deals with the description of mixtures of complex materials, as they occur in biological organisms. (*Problem 5*) How should we have to modify the general model-building framework above to have a theoretical tool able to furnish specific models of mixtures of materials with interacting or non-interacting microstructures?

So far we have discussed just the isothermal framework. In the non-isothermal case, even just in describing rigid conductors, we know the problem of infinite speed of temperature disturbances emerging when we accept Fourier's law. Related discussions on possible phenomenological changes of Fourier's law to avoid the physical drawback populate the literature (see the critical survey [60]). (*Problem 6*) Can we say that the evident finite speed propagation of temperature disturbances depends on the influence of the material microstructure, irrespective of its type? I believe that an answer could be given by considering ν as a function of the temperature, once we have a notion of temperature far from equilibrium.

9. On the nature of mathematical models of the phenomenological world

Previous discussions express implicitly a question: *What do we do from a philosophical viewpoint when we propose a model, precisely a mathematical model in mechanics?* Summarizing some notions already discussed here helps us at least in delimiting the scenario. A body, we know, can suffer recoverable and/or permanent strain. It can be damaged, the statement making sense once we define a state that we decide be the undamaged reference. Damage can localize up to form macroscopic cracks (the adjective referring to the human average perception without instruments). A body can move with respect to an observer.

Constructing mathematical models of the mechanical behaviour of bodies means describing qualitatively and quantitatively at least part of the processes listed above. *A model is in fact a representation of a phenomenon, or a class of phenomena, addressed by data but going beyond them.*

To build up a model, we do not need to be an arid reporter of a single phenomenon, but it is necessary to have sufficient imagination to evidence the possible essential aspects of the mechanical process under scrutiny, and to connect them each other.

The construction of a mathematical model of natural phenomena has something to do with the craftsmanship and, in its highest expressions, with art for the quality and the density of the aesthetic content of the model itself.

The process determining a 'vision' from which a mathematical model emerges follows a path strictly analogous to what we traditionally consider an artistic creation. It has its roots in the researcher's imagination. The logic rigour follows. A theorem is *perceived* first, even vaguely. Then we make an effort in finding its rigorous proof. This is the way a mathematician not having solely a (so to speak) 'professional' experience of his discipline acts, a mathematician which we can consider a creative scholar.

Imagination generates a vision of the world, which may reflect on social structure in different manners. If I construct a model of the phenomenological world (or at least part of it), what I represent is my world—a point of view expressed by Ludwig Wittgenstein in item 5.641 of his *Tractatus Logicus Philosophicus* (see any edition of the *Tractatus*)—in the sense that it is a descriptive choice adopted by who expresses an interpretative cataloging of the phenomena. Such a statement has to be handled with care because a superficial analysis of it would bring us to an unfruitful arbitrariness of interpretations and descriptions of the phenomena, without any distinction in terms of effectiveness, pertinence, value. With reference to the description of physical phenomena, the word *my* referred to the world has to be intended in some statistical sense. It is connected to an observer, intended as a human community, measuring physical events in a given historical period and with certain tools that are themselves the result of a preliminary interpretation of

the phenomena. Averages and fluctuations emerging from data statistical analyses address some way the state of the knowledge in a given historical period. In this sense, the statement ‘my world’ has to be intended as the knowledge humans have in a given time. The solipsism that Wittgenstein attributes to the interaction between a single human observer and the language translates to the social collectivity and manifests itself in the process of knowledge. Its limits and the phenomenological experience push the researcher to establish or to adopt principles, which indicate the limits of his speech on the topic under analysis.

Some principles appear unavoidable—the second law of thermodynamics, the energy balance, objectivity, covariance and so on—but their explicit form can be expressed in various manners in specific cases. Alternative versions of a given concept may generate different models of the same class of phenomena, and these models can even furnish, in contrast, analogous results in specific cases. Different models can also emerge from the same principles as a consequence of the introduction of subsequent technical assumptions. A problem is then the choice among models equivalent to each other in some sense.

A way to discriminate seems to be the economy in the assumptions. In William of Ockham’s work, we find implicit the suggestion to avoid multiplying without needs the bases of an interpretative analysis: what we commonly call *Ockham’s razor*. Such a viewpoint is sometimes considered as concerning the *number* of peculiar entities involved (principles or else), other times referred to their *type*. However, in using it we have to take care because the razor may generate epistemic dilemmas: it is a progressive reduction tending to an absolute minimum of concepts. Perhaps, using Ockham’s razor with reference to the entire process of knowledge, including its implicit constraints (e.g. the degree of deepness that we decide to assign to the description of what we analyse) can give more effective results.

The choice of principles addresses our speech on a class of natural phenomena. The formal expression in mathematical terms of the foundational principles adopted determines linguistic structures. In fact, mathematics is a language with a singular peculiarity: it allows us to express statements that are at the same time qualitative and quantitative without resorting to structures of other languages. For example, when we affirm, e.g., that *the readers of this article will be at most five*, we are using English and we qualify the persons involved in our statement—*readers*—but to quantify them we resort to a concept—the number *five*—pertaining to mathematics. This peculiar aspect furnishes some indications on the descriptive effectiveness of mathematics in representing nature.

In item 4.21 of his *Tractatus*, Wittgenstein claims that what in a language expresses itself we cannot express through the language. To allow our thoughts to represent ‘reality’, it is necessary that the elements composing the propositions we express about one another be in the same relationships occurring among the elements of the reality (see item 2.15 in the *Tractatus*). This is also Pierre Hadot’s interpretation of Wittgenstein’s concept of *logic form* [61]. And the reality is for an observer what emerges in the observation. The observation imparts logic form to recorded phenomena. Our data are filtered from the beginning by our brain as observers and designers of new experiments. Also mathematics has its origin in the human brain: it emerges from our instinctive will of ordering and counting things in a process going naturally towards the construction of more and more abstract forms, its grammatic structures in the end. It is just this aspect—I believe—the source of the effectiveness of mathematics in describing the phenomena recorded in experiments. Such effectiveness is then not so much connected with the description of the world as it pertains to what we observe and to us *is* the world. The observation is organized and managed by our brain, which is also the place from which the structures constituting mathematics emerge. The natural bridge between observation and model is the thought: there we establish not only the logical form of the observation of phenomena but also the form of the language through which we describe the world. In this sense, we can interpret the early Wittgenstein when he affirms that *the limits of my language are the limits of my world* (see item 5.6 in the *Tractatus*), i.e. the limits of description and interpretation of what we perceive through senses and instruments, although the construction of an instrument presupposes a preliminary conceptual idea on some aspects of the world. The limits of the speech about

physical events are those implied by principles and mathematics adopted. They are also the limits of researcher's imagination, which determines value and would like to embrace the world trying to perceive (perhaps we cannot do nothing more than trying) its ultimate essence. For these reasons, I find unfruitful polemic positions about the presumed excessive use of mathematics in mechanics. It is not so much a matter of showing to the community the personal ability of managing articulated mathematical structures as the basic fact that when we use some tools we are able to tell something with a certain deepness and when we change tool we are telling something else, perhaps less comprehensive for being less general (this is the reason, e.g., pushing me to choose above to work with abstract differentiable manifolds instead of considering more simply \mathcal{M} as a linear space ...but this is just a trivial example). The question is to decide about what we want to tell, not *a priori* about the mathematical tool we want to use. Formal simplicity must be preferred to a more involved structure only when we reach the same level of descriptive richness with respect to *potential* events in a specific class. By contrast, manifest idiosyncrasy for advanced formal structures could be interpreted just as a way of saving your own position without entering into a land in which one believes (perhaps even unconsciously) to be unable to walk. So, the question becomes psychological more than objective. By contrast, the concrete question is the quality of the results we get and the way they are evaluated. Evaluation of models and articulate theoretical views is matter of culture, psychology, ethics of the evaluator; it is matter of time, perhaps the true riddle, and it is not an easy task, above all when we are not in front of the research academic routine, based at times on almost imperceptible variations of what we know, a routine essential otherwise to dig up the ground, hoping for flowers and fruits.

10. Creativity in mechanics

I have already mentioned craftsmanship and art in connection with the construction of mathematical models of natural phenomena—and here I think primarily of continuum mechanics of materials. I believe that my claim has general character connected with doing mathematics in a creative manner, indicating as creativity the attitude to attempt extending the domain of mathematics by introducing new concepts, proving non-trivial theorems, constructing further effective mathematical models of the phenomenological world. With 'extension of the domain' I mean the enlargement of the mathematical knowledge by *addition*, not properly a progress rendering stale what has been done previously. I do not want to discuss the problem whether the mathematical results are discoveries or creations. The ontological answer we give whatever, for a scholar trying to do mathematics in a way that we can define creative in the vague sense above, the question has no special interest. Who works this way inside mathematics considers doing it as a creative act. Commonly, nobody asks whether the *Ode to Joy* is a discovery or formulates the same question for the whole *Ninth Symphony*, or the *Goldberg Variations*, the *Cello Suites*, or the *Jupiter* symphony, just to list some examples. Although these musical masterpieces are implicit in the manifold of possible combinations of the notes on the pentagram, we all believe that their writing is a creative act and we can say they are art, even if the definition of art is a matter of disputations. In fact, we are culturally educated to think that they are art but also, instinctively, in listening to them we perceive 'something' we cannot define explicitly and we go in some sense beyond the notions we have. Implicitly, these masterpieces indicate even the constitutive nature of art: as it is the matter that defines in a sense the physical space perceived by the human observer around himself, so the works are those indicating—without avoiding ambiguity in the definition—the nature of the aesthetic experience. We can agree with Luigi Pareyson that there is possibility of art in the entire human diligence in the sense of the formativeness of our actions. Such a possibility expresses itself in the ability of performing a piece of work 'in a way extremely singular and personal, unmistakable though paradigmatic, and where we can speak about style, we have to speak of art' (my translation of the Italian original in [62, p. 64]). Then the question, in mathematics as in all the other human creative activities, is the level of the aesthetic content, its density in a work and the permanence in time of the work itself. It is not simply a question

of getting something down to a fine art, i.e. applying in rigorous and impeccable manner known techniques. Rather it is matter of adopting some available techniques and inventing new ones in order to create something inimitable for it is unique and imitable for it is a potentially unavoidable influencing reference. We can list several examples and we can quite affirm that the research in mathematics nourishes itself and is addressed by such duplicity.

Questions emerge. In fact, in defining creativity according to the indications at the beginning of this section, we need some clarifications. What is the meaning of new? Does 'new' refer to a not-previously existing concept, or else to a not-previously accepted or imagined use of an existing concept or interpretation of it? Is there any unquestionable definition of non-triviality or else is it matter of the evaluator's imagination and culture? When is a model concretely effective?

The evident possibility of ambiguity and/or incompleteness in proposing answers to the previous questions exposes who would like to delineate exactly the boundaries of creativity, in particular in mechanics, with a formal scheme to the concrete risk of constructing it just on an implicit self-referential inconsistent dream.

We do not know exactly what creativity be but we can say that it includes the ability of go through (even just rather) unexplored lands or to look in an unusual way (and the adjective implies different modulations corresponding to various degrees of creativity, whatever it be) to existing results or already debated topics. It includes the clear connection between the physical essence of the concepts considered and their mathematical expression. It is a sort of light on the phenomenological world. Should it be present, it emerges in time although it could be unrecognized in its first appearance, or, in contrast, opposed just because recognized (and in this case it is matter of opposer's psychology).

11. Praising a friend on the occasion of his 90th birthday

In the period I was working on this issue of the *Philosophical Transactions of the Royal Society*, during October 2015, I participated in a party in Gianfranco Capriz's home, organized for his 90th birthday. I was in the garden when I started to speak with some gentle persons I did not know—they were Capriz's relatives not involved in scientific research in their professional activity. One of them asked me the nature of Capriz's work and I tried to popularize its essence, being conscious that often popularization reduces to a shadow theatre of a shadow theatre. Then that person asked me how I could indicate Capriz in the community of continuum mechanics. I watched Gianfranco far in the garden with a number of former students around and after a while I answered that I consider him one of the most creative scholars in theoretical continuum mechanics I have known so far. I justified my evaluation with his continuous, still energetic and lucid, effort to go deeply inside the foundations of continuum mechanics, exploring the limits of available formulations and trying to go beyond them on the basis of physical views, even staggering, leaning against a not completely defined vision, with the consciousness that the foundational work has essential character. I also justified my evaluation with the variety of his work, which pictures him both as a problem-solver and proponent of comprehensive theories with far reaching vistas, having influence more extended than commonly declared. In summary, he has and has had a non-trivial ideas in mechanics, where I intend non-triviality as the possibility of producing non-standard fruits. And I ended the discussion remembering that if you ask Capriz to indicate one of the most creative scholars in theoretical continuum mechanics he knows, he would mention (as he did in personal conversations) Jerald L. Ericksen, for analogous reasons, being far from any idea of praising himself.

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