



Review

**Cite this article:** Mariano PM. 2024Topological features in continuum mechanics: from simple to complex bodies. *Proc. R. Soc. A* **480**: 20230919.<https://doi.org/10.1098/rspa.2023.0919>

Received: 11 December 2023

Accepted: 1 October 2024

Subject Category:

Mathematics

Subject Areas:

mathematical physics, mechanics, thermodynamics

Keywords:

continuum mechanics, defects, complex bodies, microstructures, phase fields, multi-field descriptions

Author for correspondence:

Paolo Maria Mariano

e-mail: paolomaria.mariano@unifi.it

Topological features in continuum mechanics: from simple to complex bodies

Paolo Maria Mariano

DICEA, Università di Firenze, via Santa Marta 3, Firenze I-50139, Italy

PMM, 0000-0002-3841-8408

Topological features have a ubiquitous influence on the behaviour of condensed matter, from the qualitative analysis of fluids flows to the classification of defects in simple and complex solids. We review results concerning the incidence of topological features on foundational aspects of the mechanics of simple and complex bodies, with particular emphasis on the mechanics of defects. Pertinent to this last issue, unusual concepts such as the relative power or the structure invariance of the Clausius–Duhem inequality under diffeomorphism-based observer changes are discussed.

1. Introduction

Nondum matura est.

Phaedrus (4, 3, 4) from Aesop (15 ab Hausrath)

In the standard format of continuum mechanics, the morphology of a body is described only by a fit region \mathcal{B} of the Euclidean space. No geometric information is given about the low-spatial-scale material morphology. The description of defects is only limited to the geometry of \mathcal{B} . When microstructural events influence the gross behaviour, the description of the body morphology needs to be enriched: we introduce phase fields that (generically) take values on a differentiable manifold, say \mathcal{M} . The topological properties of \mathcal{M} furnish further information on the defect structures. But there is something more of fundamental character about the paradigm: such fields are considered to be observable so that true interactions are associated with them. Thus, the classical notion of observer has to be refined.

Another question deals with the balance equations, above all those of microstructural interactions associated with the ‘mechanisms’ described by the phase fields, and those that involve actions driving the evolution of defects at macroscopic scale: are these balances first principles? We may postulate them in analogy with those of macroscopic momentum and moment of momentum. However, analogy is only a hope, to be perhaps adopted only as a starting point that requires subsequent proofs and justifications. Thus, a question remains: can we derive such a balances from a more primitive source? Answering this opens the way to reliable generalizations. My answer to this last question is in the affirmative.

In discussing reasons for the answer, we find it natural to consider how topological features influence the scenario. They are often primarily referred to the analysis of fluid flows since Arnold’s 1966 pioneering work on the hydrodynamics of perfect fluids in the light of infinite-dimensional Lie groups [1]. Not restricted to fluid flows, topological features have, however, ubiquitous incidence on the mechanical behaviour of condensed matter.

We refer those interested in the topology of fluid flows to the elegant and comprehensive treatise [2]. Here, instead, we look at results concerning general foundational issues and the mechanics of defects in simple and complex bodies. The adjective *complex* as referred to bodies is used to recall in short that they are made of condensed matter in which microstructural events at low spatial scale(s) influence the gross behaviour in a way hardly representable in the traditional format of continuum mechanics.

The classical paradigm was clarified and set up during the second half of twentieth century [3–6]. Its well-known structure is as follows:

- A body is considered to be a set of so-called material elements, each intended as a cluster of atoms not otherwise specified. The body morphology is represented by a fit region in the Euclidean space. So, material elements are considered as indistinct pieces of matter identified by points.
- To be defined, a deformation requires the choice of a reference configuration, selected in a space that is a copy of the physical space for reasons that will be clear later. Every deformation is assumed to avoid self-penetration of matter, to be differentiable, one-to-one and such that it preserves the space orientation.
- Every part (itself a fit region) of a body interacts with adjacent parts and the rest of the universe. Interactions are linear functionals over an algebra of bodies, and are subdivided into bulk and surface families that are balanced.
- Balance equations of standard forces and couples refer to those bodies whose morphology is represented as above.
- The type of material is specified by state functions—constitutive structures—that are restricted by the Clausius–Duhem inequality, a version of the second law of thermodynamics. The role assigned to the second law is to be a source of admissibility conditions for constitutive structures, stability and propagation of discontinuities as shock waves.

Considering material complexity induced a shift in such a paradigm. The main features of the associated general model-building framework are as follows:

- Every material element is considered as a system with own structure. The body morphology is represented not only by a fit region in space but also by *additional* descriptors of the microstructural morphology (phase fields). Generically, we take such fields as valued on a finite-dimensional manifold, say \mathcal{M} , considered *not* embedded into a linear space. Special choices of \mathcal{M} depend on specific physical circumstances.
- These additional descriptors are considered as observable entities. This requires an extension of the classical notion of observer.
- Interactions are associated with *every* kinematic mechanism foreseen by the geometric representation of the body morphology. Thus, microstructural interactions emerge.
- The pertinent balance laws can be derived from invariance principles, together with the standard balances of forces and couples. So, they do not need to be postulated.

- The Clausius–Duhem inequality can play a classical role, and even a new one that we also discuss here.

Appropriate references are introduced later. Here, we only summarize the structure of this paper.

In §2, we begin by recalling for future use the classical Cauchy stress theorem, written with reference to a generic balance law (not necessarily the classical integral balance of forces). With respect to traditional treatments introduced even at undergraduate level, the version recalled here points out that weaker regularity than the one in standard textbooks is sufficient for the result. This opens the problem of how ‘wild’ from a topological viewpoint the geometrical representation of macroscopic configurations can be, and how contact interactions depend on a non-smooth choice of a body part (another topological feature). Some answers are provided in §3, where (say) edge interactions are considered. Accounting for them, at least to some extent, requires variations in the algebra of bodies as introduced by Noll [3,7,8] to define interactions. Further changes are necessary when we consider microstructural events with the actions driving and connecting them with the macroscopic behaviour. To define such actions it seems useful to extend a different approach to interactions still proposed by Noll [8,9], who did not account for microstructures. Before going into details, however, we need to discuss how accounting for material complexity starts from a refined representation of the body morphology. This is done in §4 to §6. Topological methods allow a classification of defects at various scales, and with reference to different material structures. An extension of the notion of observer is also implied, as discussed in §7. Then, in §8, we define microstructural actions in terms of the external power that they perform and explain also the notion of *relative power*, which is also relevant in the presence of growing defects. In particular, we show how a requirement of objectivity for the relative power implies the deduction of standard, microstructural and configurational actions. Inertial effects are discussed in §9. Thermodynamic aspects are summarized in §10. A requirement of structure invariance for the Clausius–Duhem inequality under diffeomorphism-based observer changes becomes a source of all basic ingredients of a continuum model. Section 11 collects miscellaneous material and indicates perspectives.

Editorial restrictions in length do not allow us to render self-contained the paper. Readers are presumed to be literate in some aspects of topology, differential geometry, mathematical analysis and to be familiar with continuum mechanics. In any case, indications of pertinent treatises are provided to allow appropriate further readings. This paper discusses primarily ideas that are often unusual; they have a foundational character.

2. General fluxes

Let \mathcal{B} be an open connected set with Lipschitz boundary in \mathbb{R}^k . A *proper domain* (or *part*) \mathfrak{b} of \mathcal{B} is any open bounded subset with non-zero volume and Lipschitz boundary. Consider a (say) scalar *extensive* entity on any proper domain \mathfrak{b} of \mathcal{B} . It is characterized by a *production* $\mathcal{R}(\mathfrak{b})$ and a *flux* $\mathcal{Q}(\partial\mathfrak{b})$ across the boundary $\partial\mathfrak{b}$. Commonly, a balance law is a prescription that the production equals the pertinent flux, namely

$$\mathcal{Q}(\partial\mathfrak{b}) = \mathcal{R}(\mathfrak{b}). \quad (2.1)$$

Requiring that production and flux are extensive means that they are additive over disjoint subsets. Specifically, \mathcal{R} is naturally endowed with the structure of a measure, that is a set function that vanishes on the empty set and is countably additive over disjoint subsets, those constituting a σ -algebra in a given space. Specifically, we take for \mathcal{R} a signed *Radon measure*, that is a measure such that its value $\mathcal{R}(\mathfrak{b})$ is the supremum over values computed on all compact sets

$K \subset \mathfrak{b}$, and every point $x \in \mathfrak{b}$ has a neighbourhood \mathcal{I}_x with finite measure. Linear functionals such as

$$\rho \mapsto \int_{\mathfrak{b}} \rho \, dx,$$

defined over locally compact topological spaces (as \mathbb{R}^n is) correspond to Radon measures. We also choose \mathcal{Q} to have density $\hat{f}_{\partial\mathfrak{b}} \in L^1(\partial\mathfrak{b})$, with respect to the $(k-1)$ -dimensional Hausdorff measure \mathcal{H}^{k-1} ; for any domain \mathfrak{C} of $\partial\mathfrak{b}$, the flux \mathcal{Q} through \mathfrak{C} is given by

$$\mathcal{Q}(\mathfrak{C}) := \int_{\mathfrak{C}} \hat{f}_{\partial\mathfrak{b}}(x) \, d\mathcal{H}^{k-1}(x).$$

Theorem 2.1. (Cauchy's flux theorem) [10, p. 3]. With the above assumptions, let $|\hat{f}_{\mathfrak{b}}(x)| \leq K$ for some constant K for any $x \in \partial\mathfrak{b}$ and all proper domains \mathfrak{b} . With each \mathfrak{n} in the $k-1$ sphere S^{k-1} is associated a bounded measurable function $\mathfrak{a}_{\mathfrak{n}}$ on \mathcal{B} with the following property: given \mathfrak{b} , suppose that x is a point in $\partial\mathfrak{b}$ such that the normal to \mathfrak{b} exists and is \mathfrak{n} . Assume also that x is a Lebesgue point for $\hat{f}_{\mathfrak{b}}$ with respect to \mathcal{H}^{k-1} , and that the upper derivative of $|\mathcal{R}|$ at x , with respect to Lebesgue measure, is finite. Then,

$$\hat{f}_{\partial\mathfrak{b}}(x) = \mathfrak{a}_{\mathfrak{n}}(x),$$

meaning that $\hat{f}_{\mathfrak{b}}$ depends on $\partial\mathfrak{b}$ only through the normal \mathfrak{n} . Also, there exists a vector field $\mathfrak{a} \in L^{\infty}(\mathcal{B}; \mathbb{M}^{1 \times k})$, with $\mathbb{M}^{1 \times k}$ the linear space of $1 \times k$ matrices, such that, for any fixed $\mathfrak{n} \in S^{k-1}$

$$\mathfrak{a}_{\mathfrak{n}}(x) = \mathfrak{a}(x) \cdot \mathfrak{n}$$

almost everywhere in \mathcal{B} . Finally, the vector function \mathfrak{a} satisfies the field equation

$$\operatorname{div} \mathfrak{a} = \mathcal{R}$$

in the sense of distributions on \mathcal{B} .

Theorem 2.1 holds even when $\hat{f}_{\partial\mathfrak{b}}$ takes values in a more general linear space (say) X . So, when **balance (2.1)** is the integral balance of forces, the linear operator $\mathfrak{a}(x)$ coincides with the standard stress.

Are there non-trivial physical motivations for looking at a generality such as the one in Theorem 2.1, or does the smooth case suffice? Formulating an answer requires us to look at least approximately to the way ideas about the representation of contact interactions evolved historically.

3. Topology influences the representation of contact interactions: the classical case

In his first derivation of the stress tensor, Cauchy considered *smooth* ideal cuts dividing a body into disjoint parts. His smoothness assumption does not cover topological features such as shocks, corners and edge contact of bodies. Something more is needed to account for these aspects. Related questions are as follows: how can the (possibly variegated) nature of contact interactions be effectively described with simple motivated hypotheses? What are a body *and* an appropriate class of body parts? The first question pertains to properties of the mapping describing interactions. The second question is related to the domain on which interactions are defined.

Physics suggests that a contact interaction should be additive with respect to disjoint components of $\partial\mathfrak{b}$. The complement of \mathfrak{b} in \mathcal{B} should also be a body part. Consequently, the set \mathcal{B}^{sub} of parts \mathfrak{b} of \mathcal{B} could be reasonably supposed to be closed under finite union, finite intersection and the complement of its elements.

Difficulties emerge. If $\mathfrak{b} \in \mathcal{B}^{sub}$, itself \mathfrak{b} should contain its boundary; otherwise speaking of a common boundary between two body parts in contact would lose meaning. However, as complements of closed body parts we find *open* sets, so that making a representation of interactions we have to decide whether open body parts can exert a contact interaction on each other, and whether it might be the same as that for the corresponding closed body parts. Implicit is the assumption that the role of body parts in contact is always interchangeable. Then, the emerging structure for \mathcal{B}^{sub} is the one of a Boolean algebra. Such a structure is at the roots of Noll's representation of interactions. They are subdivided—we know—into bulk and contact families, both represented by vector-valued measures defined on Borel subsets of each body part [7]. Specifically, global standard bulk and contact actions are assumed to be, respectively, given by the integrals

$$\int_{\mathfrak{b}} b^{\dagger} d\mu(x) \quad \text{and} \quad \int_{\partial\mathfrak{b}} t_0 d\mathcal{H}^{k-1}(x),$$

where b^{\dagger} is the sum of inertial (b^{in}) and non-inertial (b) components, and the densities b^{\dagger} and t_0 are bounded, that is, there are constants C_1 and C_2 such that $|b^{\dagger}(x)| < C_1 < +\infty$ and $|t_0(x)| < C_2 < +\infty$. Continuity is presumed for t_0 .

In 1968 Gurtin *et al.* [11] were able to prove Cauchy's theorem by requiring only that t_0 is integrable. More precisely, they looked at global fluxes, say \mathcal{Q} , presuming their boundedness, that is, $|\mathcal{Q}(\hat{S})| \leq C \text{area}(\hat{S})$ and $|\mathcal{Q}(\partial\mathfrak{b})| \leq C \text{vol}(\mathfrak{b})$ for all oriented surfaces \hat{S} and all body parts \mathfrak{b} , with C a constant.

Also, if we consider body parts as closures of open (compact) sets with piecewise smooth boundary, such a family is *not closed* under intersection. So, Noll [8] discussed physically acceptable requirements for a family of bodies or body parts of a given body, based on a set Ω , called a *material universe*, endowed with a preorder relation $<$, read as *being part of*.

Write $\mathfrak{A}, \mathfrak{B}, \mathfrak{C}$ and \mathfrak{D} for elements of Ω . Given $\mathfrak{A}, \mathfrak{B} \in \Omega$, there can be at most one $\mathfrak{C} \in \Omega$ such that $\mathfrak{C} < \mathfrak{A}, \mathfrak{B}$ and $\mathfrak{C}' < \mathfrak{A}, \mathfrak{B} \implies \mathfrak{C}' < \mathfrak{C}$. If such \mathfrak{C} exists, it is what we call the *greatest common part* of \mathfrak{A} and \mathfrak{B} ; for it we write $\mathfrak{C} = \mathfrak{A} \wedge \mathfrak{B}$. Given $\mathfrak{A}, \mathfrak{B} \in \Omega$, there can be at most one $\mathfrak{D} \in \Omega$ such that $\mathfrak{A}, \mathfrak{B} < \mathfrak{D}$ and $\mathfrak{A}, \mathfrak{B} < \mathfrak{D}'$ implies $\mathfrak{D}' < \mathfrak{D}$. If such a \mathfrak{D} exists, we call it the *least envelope* of \mathfrak{A} and \mathfrak{B} writing $\mathfrak{D} = \mathfrak{A} \vee \mathfrak{B}$. These operations endow Ω with a *lattice* algebraic structure. It is defined by a number of axioms [7,8]: (i) $\mathfrak{A} = \mathfrak{B}$ if and only if $\mathfrak{A} < \mathfrak{B}$ and $\mathfrak{B} < \mathfrak{A}$. (ii) $\mathfrak{A} < \mathfrak{B}$ and $\mathfrak{B} < \mathfrak{C} \implies \mathfrak{A} < \mathfrak{C}$. (iii) There are two elements, namely \emptyset and ∞ in Ω , called the *material nothing* and the *material all*, such that $\emptyset < \mathfrak{A} < \infty$ for all $\mathfrak{A} \in \Omega$. (iv) For each $\mathfrak{A} \in \Omega$, there is exactly one $\mathfrak{A}^e \in \Omega$, called the *exterior* of \mathfrak{A} , such that $\mathfrak{A} \wedge \mathfrak{A}^e = \emptyset$ and $\mathfrak{A} \vee \mathfrak{A}^e = \infty$. (v) If $\mathfrak{A} \wedge \mathfrak{B}^e = \emptyset$, $\mathfrak{A} < \mathfrak{B}$. (vi) For all $\mathfrak{A}, \mathfrak{B} \in \Omega$, $\mathfrak{A} \wedge \mathfrak{B}$ exists.

Write $(\Omega \times \Omega)_{sep}$ for the set $(\Omega \times \Omega)_{sep} := \{(\mathfrak{A}, \mathfrak{B}) \in \Omega \times \Omega \mid \mathfrak{A} \wedge \mathfrak{B} = \emptyset\}$. A mapping $t_n : (\Omega \times \Omega)_{sep} \rightarrow \mathcal{V}$, where \mathcal{V} is some vector space, is called an *interaction* if $t_n(\cdot, \mathfrak{A}^e) : \Omega \rightarrow \mathcal{V}$ and $t_n(\mathfrak{A}, \cdot) : \Omega \rightarrow \mathcal{V}$ are additive for every $\mathfrak{A} \in \Omega$. An interaction t_n satisfies the *law of action and reaction*, namely $t_n(\mathfrak{A}, \mathfrak{B}) = -t_n(\mathfrak{B}, \mathfrak{A})$ for all $\mathfrak{A}, \mathfrak{B} \in \Omega$, with $\mathfrak{A} \wedge \mathfrak{B} = \emptyset$, if and only if the mapping $\mathfrak{A} \mapsto t_n(\mathfrak{A}, \mathfrak{A}^e)$ is additive [12]. A question remains: what types of sets in the Euclidean space can we put in one-to-one correspondence with the elements of Ω ?

In 1976, Gurtin & Martins [13] noticed that polyhedra satisfy Noll's axioms. Thus, they considered fluxes as additive mappings over polyhedral surfaces. The question was: why only polyhedra? Indeed, in 1969 Kirby & Sebermann [14] discovered manifolds without polyhedral structure. And there is no *a priori* reason to avoid them if, according to Truesdell, we consider bodies as manifolds. In fact, what we have to understand is *how rich a system of body parts should be*.

Banfi & Fabrizio in 1979 [15] and Ziemer [16] in 1983 found that sets of finite perimeter satisfy Noll's axioms; they are endowed with a normal almost everywhere on their measure theoretic boundary. They could be, however, too exotic with respect to physical acceptability as sets that may represent tangible bodies. Thus, Gurtin *et al.* [17] reduced in 1986 the class by choosing sets that coincide with their measure theoretic interior. Such a class, however,

appeared too narrow. So, in 1988, Noll & Virga [18] proposed to adopt the so-called *fit regions* (bounded regularly open sets with negligible boundary), which are somewhere in between the previous classes. They exploited De Giorgi's idea of sets with reduced boundary [19]. Once the notion of a fit region was accepted, in question was the analysis of interactions on this type of sets.

In 1991, M. Šilhavý [20] (see also [21]) extended Cauchy's theorem to fluxes for which, with \mathcal{Q} an additive functional over oriented disjoint surfaces, L^p -functions f_1 and f_2 exist and are such that, for $p \geq 1$,

$$|\mathcal{Q}(\hat{S})| \leq \int_{\hat{S}} f_1 d\mathcal{H}^{k-1}(x) \quad |\mathcal{Q}(\partial\mathfrak{b})| \leq \int_{\mathfrak{b}} f_2 d\mu(x),$$

for any oriented surface \hat{S} in a body. The last inequality mimics in a certain sense the balance of standard forces. De Giovanni *et al.* [22] proposed in 1999 to replace the absolutely continuous volume measure corresponding to f_2 in Šilhavý's work with an arbitrary Radon measure. Consequently, in the representation of contact interactions they were naturally prompted to consider tensor fields with divergence a measure. Chen & Frid [23], Chen & Torres [24] also Šilhavý [25] refined the result.

In this setting, *what about forces concentrated at a point?* They are an idealization, indeed. However, accounting for them, as in common undergraduate classroom exercises, requires a careful refinement of the theory. The reasons are as follows.

Consider a rectangular slab subjected to an in-plane single force orthogonal to one side and located at its middle point. To accord with Cauchy, imagine to cut ideally the slab along a straight line coinciding with the force direction. We have no criterion to decide whether this point belongs to the left- or right-hand cut piece. Should we consider it twice or imagine it disappears? Both choices are inconsistent with the physical evidence of the additive character of forces [26]. The associated stress field admits a measure as divergence with a concentration at the force application point. We can compute the traction exerted in small cones with vertices at that point. However, a Cauchy flux defined on surfaces seems incapable of describing such a situation with in detail. A way to account for the situation was indicated in 2007 by Schuricht [27], who weakened the assumption that two continuous interacting bodies should be interchangeable and assumed that, in general, $\iota_n(\mathfrak{A}, \mathfrak{B}) \neq \iota_n(\mathfrak{B}, \mathfrak{A})$. He maintained the physics-based assumption that ι_n is additive over disjoint body parts \mathfrak{b}_1 and \mathfrak{b}_2 , while requiring that countable additivity can be employed only for $\iota_n(\cdot, \mathfrak{b}_2)$. Schuricht assumed that the role of a body part \mathfrak{b}_2 exerting an action over \mathfrak{b}_1 differs from that of \mathfrak{b}_1 resisting what \mathfrak{b}_2 does. In other words, the action $\iota_n(\cdot, \mathfrak{b}_2)$ of \mathfrak{b}_2 has a different nature than the reaction $\iota_n(\mathfrak{b}_1, \cdot)$ of \mathfrak{b}_1 . With this proviso, Schuricht selected the Borel σ -algebra or a suitable sub-algebra thereof, where unions, intersections and complements are understood in the usual set-theoretic sense.

Furthermore, Noll's *principle of local action* states that the stress at a point should depend only on the response of material points within an arbitrarily small neighbourhood of it. Schuricht used it to characterize contact interactions. He postulated that the action exerted on a body part \mathfrak{b}_1 by another body part \mathfrak{b}_2 merely depends on those parts of \mathfrak{b}_2 outside \mathfrak{b}_1 that lie within an arbitrarily small neighbourhood of \mathfrak{b}_1 . Then, he required that the material corresponding to a set of measure zero cannot exert a non-trivial action and at the same point a non-trivial interaction can be detected by a reaction of the surrounding material even if we disregard the matter in a set of zero volume. A consequence is that a single material point can resist but cannot exert a non-trivial action.

For body parts \mathfrak{b} with piecewise smooth boundary, $\iota_n(\mathfrak{b}_1, \mathfrak{b}_2)$ exerted on \mathfrak{b}_1 by \mathfrak{b}_2 can be represented as

$$\iota_n(\mathfrak{b}_1, \mathfrak{b}_2) = \int_{\partial\mathfrak{b}_1 \cap \partial\mathfrak{b}_2} Pn d\mathcal{H}^{k-1}(x),$$

where P is the first Piola–Kirchhoff stress and n the normal to $\partial\mathfrak{b}_1 \cap \partial\mathfrak{b}_2$. This standard formula can be extended to all closed subsets in the sense of (functional) normal traces. However, we can define $t_n(\mathfrak{b}_1, \mathfrak{b}_2)$ in less straightforward cases because, now, t_n is defined on all Borel sets so that the necessary generalized counterpart of the previous formula is $t_n(\mathfrak{b}_1, \mathfrak{b}_2) = (\text{Div}P_{\mathfrak{b}_2})(\mathfrak{b}_1)$, with

$$P_{\mathfrak{b}_2} := \begin{cases} P & \text{on } \mathfrak{b}_2 \\ 0 & \text{otherwise.} \end{cases}$$

$\text{Div}P_{\mathfrak{b}_2}$ has to be intended as a measure for all $\mathfrak{b}_1 \in \mathcal{B}^{sub_1}$ and $\mathfrak{b}_2 \in \mathcal{B}^{sub_2}$, where $\mathcal{B}^{sub_2} \subset \mathcal{B}^{sub_1}$ is a suitable sub-algebra. Neither surfaces nor normal vectors enter the representation of interactions in this way, because fluxes are not exploited.

4. The manifold \mathcal{M} of microstructural shapes

When we discuss observer changes, we often declare or find written in textbooks that different observers perceive the same reference configuration \mathcal{B} . However, an observer change involves the whole ambient space. Thus, since \mathcal{B} is not restricted to a point, its representation should then change. To avoid the contradiction, we can select two isomorphic copies of the physical space, namely \mathbb{R}^k and $\tilde{\mathbb{R}}^k$, with the isomorphism $\iota: \mathbb{R}^k \rightarrow \tilde{\mathbb{R}}^k$ chosen to be simply the identification.

(a) A few notes on a standard matter

From now on, we set $k = 3$ for the sake of simplicity. Deformations are one-to-one, differentiable and orientation preserving maps $\mathcal{B} \ni x \mapsto y := \tilde{y}(x) \in \tilde{\mathbb{R}}^3$. A metric g is (or can be) naturally defined over \mathcal{B} . It is what we call a *reference metric*. After we assign a basis $\{\mathbf{e}_A\}$, $A = 1, 2, 3$ in \mathbb{R}^3 , with dual basis $\{\mathbf{e}^A\}$, we have $g = g_{AB}\mathbf{e}^A \otimes \mathbf{e}^B$, where \otimes indicates the standard tensor product. Every element of $\{\mathbf{e}^A\}$ is defined to be such that $\mathbf{e}^A \cdot \mathbf{e}_B = \delta_B^A$, where δ_B^A is the Kronecker symbol and the interposed dot indicates standard duality pairing, that is, $\mathbf{e}^A(\mathbf{e}_B) := \mathbf{e}^A \cdot \mathbf{e}_B$, because \mathbf{e}^A is a linear form. Also, g may be connected with peculiar material features; for example, when we look at periodic crystals, choices of a local basis may indicate peculiar features of the atomic lattice [28]. Another metric, say \tilde{g} , is assigned arbitrarily to the ambient physical space $\tilde{\mathbb{R}}^3$. We have $\tilde{g} = \tilde{g}_{ij}\tilde{\mathbf{e}}^i \otimes \tilde{\mathbf{e}}^j$, with $\tilde{\mathbf{e}}^i$ the generic i -th element of a dual basis in $\tilde{\mathbb{R}}^3$; \tilde{g} may or not be coincident with g . When defects intervene at crystal scale or at molecular scale, depending on the type of bodies, a way of representing their effects on the reference configuration is to consider a time-varying metric [29]. However, such an approach refers essentially to defects that alter the structure we have chosen to be associated with g ; it does not cover the occurrence of defects such as cracks. Thus, in general we need something different such as *time-varying* (known also as *parameterized* or *mutant*) reference configurations (see, e.g. [30]).

F is the derivative $F := D\tilde{y}(x)$, so it is the linear operator expressing the tangent map associated with the deformation. The gradient $\nabla\tilde{y}(x, t)$ (a covariant derivative) is also well-defined; its definition requires the existence of a reference frame in which $\nabla y = \nabla\tilde{y}(x) = (\frac{\partial y^j}{\partial x^i})^A \tilde{\mathbf{e}}_i \otimes \mathbf{e}_A$. In this frame of reference, ∇y and Dy are related by $(\frac{\partial y^j}{\partial x^i})^A g_{AB} = (Dy)^i_B$; so, they can be identified when g_{AB} coincides with δ_{AB} , that is, the Kronecker's symbol with covariant components. For this reason, we continue to call F a *deformation gradient*; F maps linearly the tangent space $T_x\mathcal{B}$ to \mathcal{B} at x on to the analogous space $T_{\tilde{y}(x)}\mathcal{B}_c$ and we write in short $F \in \text{Hom}(T_x\mathcal{B}, T_{\tilde{y}(x)}\mathcal{B}_c) \simeq \text{Hom}(\mathbb{R}^3, \tilde{\mathbb{R}}^3)$. Two linear operators are associated with F : the *formal adjoint* $F^* \in \text{Hom}(T_{\tilde{y}(x)}^*\mathcal{B}_c, T_x^*\mathcal{B})$ and the *transpose* $F^T \in \text{Hom}(T_{\tilde{y}(x)}\mathcal{B}_c, T_x\mathcal{B})$. They coincide when both \tilde{g} and g are the (fully covariant) identity tensors, and we compute $F^T = g^{-1}F^*\tilde{g}$.

Such a classical picture does not capture shapes and related changes of several active microstructures. Additional descriptors need to be accounted for.

(b) Physically significant examples of microstructural morphology

Examples are in no significant order.

Planar spins: Each point of $\mathcal{B} \subset \mathbb{R}^2$ is endowed with a unit vector $\nu \in S^1$, so that $x \mapsto \nu := \tilde{\nu}(x) = \nu_1 \cos \theta(x) + \nu_2 \sin \theta(x)$, with θ an angle in the plane.

Ordinary spins: \mathcal{B} is now in \mathbb{R}^3 and $\nu \in S^2$.

These two schemes may represent materials undergoing polarization, such as ferroelectrics and magnetoelastic ones, under conditions of saturation. Transient states require to substitute S^1 and S^2 with B_{p_1} and B_{p_2} balls in \mathbb{R}^2 and \mathbb{R}^3 , respectively, with radii equal to the maximum admissible polarization [31].

Superfluid helium-4: ν represents a wave function; it is the value at x of a complex scalar field of fixed magnitude χ_0 but arbitrary phase $\hat{\theta}$, namely $\nu := \tilde{\nu}(x) = \chi_0 \exp(i\hat{\theta}(x))$.

Liquid crystals: They are arrangements of stick molecules with end-to-tail symmetry; in other words, each molecule can be described by a vector with no arrowhead, or one having identical arrowheads at each end. They appear in different phases (see details in [32]):

(i) *Isotropic phase*—no local preferred direction in the molecular arrangement. Introducing ν is not strictly necessary.

(ii) *Nematic phase:* we have local preferred alignments. The introduction of ν is necessary. It can be selected as a direction in the projective plane \mathbb{P}^2 [33–35], that is the unit sphere S^2 constrained by the identification of diametrically opposite points, or a dyad $\nu := n \otimes n$, with $n \in S^2$, or its traceless version $\nu := n \otimes n - \frac{1}{3} \text{tr}(n \otimes n)I$, with I the unit tensor, arranging ν to have a pair of degenerate eigenvalues [32]. If we consider ν in the projective space \mathbb{P}^2 and refer it at every x to the ‘average’ of the orientation distribution of molecules in a small neighbourhood of x , scalars may give indications at least on the first moment of the distribution. They are the *degree of orientation* [36] and the *degree of prolation* [37].

(iii) *Smectic phase:* It is a layered phase in which layers are parallel and each of them shows nematic order. In this case, we need to adopt the nematic-type description in each layer and also a parameter indicating the layer thickness (see [38,39]).

(iv) *Cholesteric phase:* There are layers with no positional ordering, but a director axis varying with layers in a way that tends to be periodic. The distance at which a 360° rotation is completed is known as the pitch. Eventually, we have a helical structure.

Biaxial nematics: The symmetry of molecules is that of a rectangular box. The natural representation for them is to choose $\nu \in SU(2)/Q8$, where $SU(2)$ is the special unitary group, while $Q8$ is the group of quaternions. It is how to use $\nu \in SO(3)/\mathcal{D}_2$, with \mathcal{D}_2 the *four* element group consisting of the identity and 180° rotations about three mutually perpendicular axes [32].

Reduced-dimension-type schemes for structural elements: A three-dimensional beam can be reduced to a one-dimensional body endowed with a field of directors, which describes the behaviour of beam cross-sections, assumed to remain rigid [40,41]. The addition of a scalar field allows one to consider cross-section warping. Other fields, defined on the beam axis can furnish information on possible additional microstructure over each cross-section (a prominent case is the one of birods [42], a beam-type scheme for DNA). Shells can be considered as surfaces with directors (see, e.g. [40,41,43]), but also additional fields may describe through-the-thickness microstructure [44].

Fluids with polymers in an emulsion: In this case, a natural choice is to consider ν as a second-rank tensor describing the independent deformation of a molecule relatively to the ground fluid motion [45].

Fluids with bubbles: ν is the volume fraction of bubbles [46].

There are even some more intricate (although natural) choices of ν .

Superfluid helium-3 in dipole locked A phase: We need a pair of distinguished orthonormal axes, arbitrarily oriented, namely a_1 and a_2 . They can be arranged into a complex vector $\nu = a_1 + ia_2$

constrained to satisfy the nilpotent conditions $\nu \cdot \bar{\nu} = 1$ and $\nu \cdot \nu = 0$, where $\bar{\nu}$ is the complex conjugate of ν ; another appropriate choice is $\nu \in SO(3)$ [47].

Superfluid helium-3 in dipole-free A phase: $\nu = n \otimes \bar{r}$ with $n \in S^2$ and \bar{r} a nilpotent vector [47].

Phase-transitions: First- and second-order phase transitions require various possible expressions for ν , depending on circumstances, according to Landau's theory [48].

Cracks, microcracked bodies and more general damage: ν could be chosen as a vector or a second-rank tensor, the second choice being appropriate for anisotropic damage, a scalar field working for the isotropic case [49].

Once we choose ν , a spatial scale λ is associated with ν , although not always rendered explicit: it is the scale at which we consider the microstructure described by ν .

(c) Defects at different spatial scales

When we limit a description of the body morphology to the sole choice of the fit region \mathcal{B} , we recognize point-like, surface-like and bulk-like defects. When we enrich the way we describe the body morphology, we can consider defects associated with the material structure described by ν .

For example, consider planar spins in two-dimensional space, described by $x \mapsto \nu := \tilde{\nu}(x) \in S^1$, a map that is continuous and differentiable everywhere in the plane, except at a point \hat{x} . Presume also to know the explicit form of ν at all x farther from \hat{x} than some distance d . We can recognize the singularity at \hat{x} avoiding information about the region below d . Take any circle centred on \hat{x} with radius larger than d , or more generally a simple closed contour. We can measure the total angle with respect to some fixed direction through which the unit vector ν turns as we proceed along the whole circular contour. Since $\tilde{\nu}$ is continuous and known explicitly on the circle, we obtain an integer multiple of 2π , say $\epsilon 2\pi$. The factor ϵ is what we call the *winding number*. It is constant when we vary the circle. Then, if ϵ is non-zero, ν turns around \hat{x} by following the circle, no matter how small the circle becomes; the derivative of ν diverges at \hat{x} . Different cases can be listed: (i) The spin field is uniform over a generic circular contour in the plane. It is therefore mapped into a single point of $S^1 = \mathcal{M}$. (ii) The spin field is non-uniform over a circular contour with zero winding number. The map on to S^1 can be shrunk to a point: it means that the singularity is removable. (iii) The spin is non-uniform with winding number 2. The map over S^1 wraps its contour twice.

In general, we can say that a zero winding number type singularity is said to be *removable* or *topologically unstable*. Singularities with non-zero winding number are called *topologically stable*. Those in the same class, each defined by a value of the winding number, are said to be *topologically equivalent*.

Defects in the same topological class can be transformed into one another by local surgery. Defects with different winding number cannot be transformed into one another by local surgery, since such a transformation requires altering the discrete winding number arbitrarily far from the singularity.

Boundary conditions may exclude smoothness of the field $\tilde{\nu}$. Consider, for example, a nematic liquid crystal at rest (or in a laminar motion) in a two-dimensional channel. We can prescribe boundary conditions by spreading surfactants on the channel walls. Assume to use on a wall a percentage of surfactant determining a certain angle of anchoring for the molecules and another percentage prescribing the mirror orientation on the other wall. Inevitably, a discontinuity appears along the channel axis.

(d) A path towards unification

At this point, a key question is whether, owing to the plurality of possible significant examples, we need to construct a plurality of specific models or we may imagine a model-building

structure so flexible and concrete as to cover all, or almost all, the above listed cases. If so, it would become a useful tool to go even beyond the above list, even tackling the description of those materials that we design to exploit a behaviour not otherwise available in nature, those that we call metamaterials.

To construct such a general model-building framework, we start by enriching the way we represent the body morphology. We thus consider at every point of the fit region \mathcal{B} the variable ν as an element of a space \mathcal{M} endowed with the structure of a differentiable manifold, without adding any further specification on ν . In this picture, ν is thus a generic coarse-grained descriptor of the material structure at a certain spatial scale λ . We write $\nu \sim O(\lambda)$ meaning that ν is of order λ . With $f(\nu, D\nu)$ a differentiable function of its arguments, we have

$$\frac{\partial f}{\partial \nu} \cdot \nu \sim O(\lambda^2), \quad \frac{\partial f}{\partial D\nu} \cdot D\nu \sim O(\lambda^2). \quad (4.1)$$

In particular, we select \mathcal{M} to be finite-dimensional, Riemannian and geodesically complete, although an infinite-dimensional manifold of measures could also be employed in specific circumstances, even if we will not discuss this last case (for the infinite-dimensional case, see [50]).

We briefly recall the definition of differentiable manifold. Connected properties are discussed in deep, elegant and erudite treatises on differential geometry (examples are [51] and [52]).

A Hausdorff topological space X with topology τ_X is said to be *locally Euclidean* with dimension m if every of its point admits a connected neighbourhood $\mathcal{U} \in \tau_X$ and a homeomorphism $\varphi: \mathcal{U} \rightarrow \mathbb{R}^d$. The pair (\mathcal{U}, φ) is a *chart*. If $x \in \mathcal{U}$ is such that $\varphi(x) = 0$, we say that the chart (\mathcal{U}, φ) specifies a local coordinate system *centred* at x . A *differentiable structure* \mathcal{F} of class C^k , with $1 \leq k \leq +\infty$, over (X, τ) is a collection of coordinate systems $\{(\mathcal{U}_\alpha, \varphi_\alpha) \mid \alpha \in \mathfrak{S}\}$, with \mathfrak{S} an index set, such that (i) $\cup_\alpha \mathcal{U}_\alpha = X$ (in other words, the coordinate systems have supports constituting a cover of X); (ii) $\varphi_\alpha \circ \varphi_\beta^{-1}$ is of class C^k for any $\alpha, \beta \in \mathfrak{S}$; (iii) if (\mathcal{U}, φ) is a chart such that $\varphi \circ \varphi_\alpha^{-1}$ and $\varphi_\alpha \circ \varphi^{-1}$ are of class C^k for every $\alpha \in \mathfrak{S}$, the inclusion $(\mathcal{U}, \varphi) \in \mathcal{F}$ holds (in short, \mathcal{F} is maximal with respect to item (ii)).

An m -dimensional *manifold* of class C^k is a pair $\mathcal{M} = ((X, \tau), \mathcal{F})$ consisting of a m -dimensional, second countable, locally Euclidean space (X, τ) with a differentiable structure \mathcal{F} of class C^k .

When we will refer to a differentiable manifold \mathcal{M} , without specifying the class, it will mean that \mathcal{M} is of class C^∞ ; in this case, we speak of a *smooth manifold*.

There are circumstances in which two different descriptors of the microstructural morphology must be considered. A paradigmatic case is the one of polarized polymer stars scattered into a melt: a vector for the polarization and a second-rank tensor for the relative strain between every polymer and the surrounding melt need to be considered. At times, even an additional scalar field can be expedient to account for the ‘radius’ of the packet zone inside the star. To describe this case, we consider \mathcal{M} as the Cartesian product of two or more manifolds, each containing a descriptor of a specific microstructural geometric feature.

Formally, let \mathcal{M}_1 and \mathcal{M}_2 be two differentiable manifolds with dimensions m_1 and m_2 , respectively; $\mathcal{M}_1 \times \mathcal{M}_2$ is a differentiable manifold of dimension $m_1 + m_2$, with a differentiable structure given by the Cartesian product of charts, namely

$$\{(\mathcal{U}_\alpha \times \mathcal{V}_\beta, \varphi_\alpha \times \varphi_\beta) \mid \varphi_\alpha \times \varphi_\beta: \mathcal{U}_\alpha \times \mathcal{V}_\beta \rightarrow \mathbb{R}^{m_1} \times \mathbb{R}^{m_2}, (\mathcal{U}_\alpha, \varphi_\alpha) \in \mathcal{F}_{\mathcal{M}_1}, (\mathcal{V}_\beta, \varphi_\beta) \in \mathcal{F}_{\mathcal{M}_2}\}.$$

5. Topology of \mathcal{M} and λ -scale defects

(a) Line defects and the first fundamental group

Let $\gamma : [0,1] \rightarrow \mathcal{M}$ be a continuous map determining a *loop* at $\nu_0 \in \mathcal{M}$, namely $\gamma(0) = \gamma(1) = \nu_0$. Its inverse γ^{-1} is defined to be $\gamma^{-1} = \gamma(1-s)$, $s \in [0,1]$. We say that ν_0 is the *base point* of the loop γ . Two loops γ and $\hat{\gamma}$ are *homotopic* if there is a continuous mapping $G : [0,1] \times [0,1] \rightarrow \mathcal{M}$ such that $G(s,0) = \gamma(s)$ and $G(s,1) = \hat{\gamma}$.

For any pair of homotopic loops γ and $\hat{\gamma}$, we define the *loop product* $\gamma * \hat{\gamma}$ as the loop $\gamma * \hat{\gamma} : [0,1] \rightarrow \mathcal{M}$ given by

$$(\gamma * \hat{\gamma})(s) = \begin{cases} \gamma(2s) & 0 \leq s \leq \frac{1}{2} \\ \hat{\gamma}(2s-1) & \frac{1}{2} \leq s \leq 1 \end{cases}.$$

The condition ‘*being homotopic to*’ is an equivalence relation. We indicate by $[\gamma]$ the equivalence class that is pertinent to γ . The set $\pi_1(\mathcal{M}, \nu_0)$ of loop equivalence classes at ν_0 complemented by the operation of loop product is a group: the *first fundamental group* of \mathcal{M} . It is said to be Abelian when $[\gamma * \hat{\gamma}] = [\hat{\gamma} * \gamma]$.

In general, $\pi_1(\mathcal{M}, \nu_0)$ depends on the base point ν_0 . However, the manifold structure of \mathcal{M} assures that it is locally path-connected. This means that every $\nu \in \mathcal{M}$ is endowed with a neighbourhood whose points can be connected with ν by arcs, since \mathcal{M} is a Hausdorff space. When \mathcal{M} is globally arc-connected, up to isomorphism, $\pi_1(\mathcal{M}, \nu_0)$ is independent of the base point and we simply write $\pi_1(\mathcal{M})$ for it.

When $\pi_1(\mathcal{M})$ is Abelian, line defects are topologically equivalent if and only if they are characterized by the same elements of $\pi_1(\mathcal{M})$. Consider two line defects associated, respectively, with γ_1 and γ_2 , two distinct elements of $\pi_1(\mathcal{M})$. If $\pi_1(\mathcal{M})$ is Abelian, the two defects can be converted into one characterized by an element γ of $\pi_1(\mathcal{M})$ that is homotopic to the loop product $\gamma_1 * \gamma_2$. They cannot be converted into one that is not homotopic to the product without having to alter the material at arbitrarily large distances.

If $\pi_1(\mathcal{M})$ is not Abelian, for the combination laws it is useful to refer to its Abelianization, namely the first homology group. It is defined as follows: let $C_1(\mathcal{M})$ be the space of all oriented cycles on \mathcal{M} , parameterized by \mathbb{R} . Let also $B_1(\mathcal{M}) \subset C_1(\mathcal{M})$ be the subspace consisting of the cycles on which the integral of closed 1-forms over such cycles vanishes (1-forms are co-vectors ξ : elements of the cotangent space of \mathcal{M} ; they are said to be closed when $d\xi = 0$, with d the exterior differential); $H_1(\mathcal{M})$ is defined to be the quotient space $H_1(\mathcal{M}) := H_1(\mathcal{M}, \mathbb{R}) = C_1(\mathcal{M})/B_1(\mathcal{M})$.

Biaxial nematic liquid crystals fall within the non-Abelian setting. This implies that line defects in such a media can cross without a connecting line except when they are two 180° disclinations of distinct type: they are, indeed, necessarily joined after crossing a 360° disclination. In turn, when $\pi_1(\mathcal{M})$ is Abelian, all line defects for the phase field can cross each other [53,54].

(b) Point defects and the second fundamental group

Point defects for the phase field can be classified by considering freely homotopic maps of spheres into the manifold \mathcal{M} . Precisely, we can define a homotopy group at $\nu_0 \in \mathcal{M}$ by considering maps $\hat{\gamma} := [0,1] \times [0,1] \rightarrow \mathcal{M}$ such that $\hat{\gamma}(0,r) = \hat{\gamma}(1,r) = \hat{\gamma}(s,0) = \hat{\gamma}(s,1) = \nu_0$. Analogous analyses to those made for defining $\pi_1(\mathcal{M})$ can be performed here: homotopic classes of spheres $\hat{\gamma}$ can be defined. Together with a product $\hat{\gamma}(s,1) * \hat{\gamma}(s,2)$, equivalence classes $[\hat{\gamma}]$ constitute the *second fundamental group* $\pi_2(\mathcal{M}, \nu_0)$ at ν_0 . When \mathcal{M} is connected, we can show that second fundamental groups at different points are isomorphic. However, the isomorphisms

between second homotopy groups based at different points are not unique, at variance of $\pi_1(\mathcal{M})$. Also, $\pi_2(\mathcal{M})$ is always Abelian [53,54].

6. Generalized motions

In the scheme that we adopt as a general model-building framework for the mechanics of complex materials, motions are intended in generalized sense. They are time-parameterized pairs of maps given by

$$(x, t) \mapsto y := \tilde{y}(x, t) \in \tilde{\mathbb{R}}^3 \quad \text{and} \quad (x, t) \mapsto v := \tilde{v}(x, t) \in \mathcal{M},$$

with $x \in \mathcal{B}$ and $t \in (t_0, t_1)$ the time. They are assumed to be at least twice piecewise differentiable with respect to t . We write \dot{y} for the Lagrangian *velocity*

$$\dot{y}(x, t) := \frac{d\tilde{y}(x, t)}{dt} \in \tilde{\mathbb{R}}^3,$$

while $v := \tilde{v}(y, t) \in \tilde{\mathbb{R}}^3$ is its *Eulerian* counterpart and we have $\dot{y} = v$. The identity does not hold for the analogous representations of the phase field time rate. Its Lagrangian representation is

$$\dot{v} := \frac{d\tilde{v}(x, t)}{dt},$$

with \dot{v} a *tangent vector* to the differentiable curve on \mathcal{M} given by $\tilde{v}(x, \cdot) : (t_0, t_1) \rightarrow \mathcal{M}$, while its Eulerian expression, precisely the time derivative of $\tilde{v}_c := \tilde{v} \circ \tilde{y}^{-1}$, is given by

$$\dot{v}_c := \frac{d\tilde{v}_c(\tilde{y}(x, t), t)}{dt} = \frac{\partial v_c}{\partial t} + (D_y v_c) \dot{y} = \frac{\partial v_c}{\partial t} + (D_y v_c) v.$$

At every $v \in \mathcal{M}$, elements of the tangent space $T_v \mathcal{M}$ can be defined in a coordinate-free way because each of them can be seen as a derivation operator. To be more precise, consider functions f and h defined on an open neighbourhood of $v \in \mathcal{M}$. We say that they have the same *germ* at v if they agree on some neighbourhood of $v \in \mathcal{M}$. This introduces an equivalence relation on C^∞ functions defined on a neighbourhood of $v \in \mathcal{M}$: two such functions are equivalent if they have the same germ. Germs associated with f and h , say \hat{f} and \hat{h} , are equivalence classes, and we denote their set at v by $\tilde{\mathcal{F}}_v$.

A tangent vector \tilde{v} at $v \in \mathcal{M}$ is a linear derivation on the algebra $\tilde{\mathcal{F}}_v$. For all germs $\hat{f}, \hat{h} \in \tilde{\mathcal{F}}_v$ and $\lambda \in \mathbb{R}$, we have $\tilde{v}(\hat{f} + \lambda \hat{h})(v) = \tilde{v}(\hat{f})(v) + \lambda \tilde{v}(\hat{h})(v)$ and $\tilde{v}(\hat{f} \circ \hat{h})(v) = \hat{f}(v) \tilde{v}(\hat{h})(v) + \hat{h}(v) \tilde{v}(\hat{f})(v)$.

The set of all tangent vectors to \mathcal{M} at v is the *tangent space* to \mathcal{M} at v , indicated by $T_v \mathcal{M}$; $T_v^* \mathcal{M}$ is its dual, the *cotangent space* of \mathcal{M} at v , that is the space of linear forms over $T_v \mathcal{M}$. Both $T_v \mathcal{M}$ and $T_v^* \mathcal{M}$ are linear, while the disjoint unions $T\mathcal{M} := \sqcup_{v \in \mathcal{M}} T_v \mathcal{M}$ and $T^* \mathcal{M} := \sqcup_{v \in \mathcal{M}} T_v^* \mathcal{M}$ are not necessarily linear. They are, respectively, the *tangent* and *cotangent bundles* of \mathcal{M} .

In what follows, we indicate by N the derivative $N := D\tilde{v}(x, t)$.

7. Observers and their changes

The enriched representation of the body morphology imposes upon us the requirement to think about the notion of observer, classically considered as a frame of reference in the physical space. In the traditional setting that space is the only one we refer to when we describe the body morphology. Here, instead, multiple spaces are involved.

Thus, an *observer* is here defined by a prescription of reference systems on *all* spaces adopted to describe the morphology of a body and its changes.

In the present setting such spaces are (i) the reference one, \mathbb{R}^3 , (ii) the physical environment, $\tilde{\mathbb{R}}^3$, (iii) the time interval (t_0, t_1) , (iv) the manifold \mathcal{M} of microstructural shapes.

Observer changes can be defined variously. Among them, first we consider a special class of those based on isometries in the physical space. They are characterized by the following properties: (i) they refer to the same timescale. (ii) They record the same reference space. (iii) They differ by time-parameterized isometries. (iv) They admit a family of differentiable homeomorphisms, namely $\mathcal{F} := \{\phi : SO(3) \rightarrow \text{Diff}(\mathcal{M}, \mathcal{M})\}$, where $\text{Diff}(\mathcal{M}, \mathcal{M})$ is the space of diffeomorphisms from \mathcal{M} on to itself.

The differentiable homeomorphisms ϕ allow one to represent over \mathcal{M} how distinct observers looking at the physical space may differently record the peculiar microstructural features described by elements of \mathcal{M} . The manifold \mathcal{M} is, indeed, only a convenient ambient to describe features of the microstructures that are in the body, that is in the physical space.

The choice of looking at a family \mathcal{F} of differentiable homeomorphisms allows us to include the case in which \mathcal{F} is empty, a case in which ν can be considered as a non-observable entity. In other words, when $\mathcal{F} = \emptyset$ we may consider ν only as a non-observable internal variable for which its evolution describes the detachment from thermodynamic equilibrium by means of phenomenological laws that do not include interactions. Such laws are not balance equations. They involve thermodynamic affinities that contribute only to the entropy production and do not play role in determining ground states.

Here, we consider \mathcal{F} as a *non-empty* set. Thus, ν is always intended as an observable entity.

Formally, let \mathcal{O} and \mathcal{O}' be two distinct observers related by isometries in the physical space. Let y be the current placement of a material point as evaluated by \mathcal{O} . The same point is for \mathcal{O}' at a place $y' = \bar{w}(t) + Q(y - y_0)$, where y_0 is a point selected at will in $\tilde{\mathbb{R}}^3$, $\bar{w}(t)$ the value of a smooth map $t \mapsto \bar{w}(t) \in \tilde{\mathbb{R}}^3$, and Q the value of a smooth map $t \mapsto Q := \tilde{Q}(t) \in SO(3)$. If \dot{y} is the velocity measured by \mathcal{O} , the other observer records a value $\dot{y}' = \dot{\bar{w}}(t) + \dot{Q}(y - y_0) + Q\dot{y}$. We pull-back \dot{y}' in the frame defining \mathcal{O} by using Q^T (a translation is not included because we consider \dot{y} as a free vector in this process). So, we define $\dot{y}^\circ := Q^T \dot{y}'$. Thus, by setting $W := Q^T \dot{Q}$ and $c = \tilde{c}(t) := Q^T \dot{\bar{w}}(t) \in \tilde{\mathbb{R}}^3$, we have $\dot{y}^\circ := c + W(y - y_0) + \dot{y}$. Since W is skew-symmetric, by definition there exists a vector-valued smooth map $t \mapsto q := \tilde{q}(t) \in \mathbb{R}^3$ such that

$$\dot{y}^\circ := c + q \times (y - y_0) + \dot{y}. \quad (7.1)$$

The counterpart of \dot{y}° over \mathcal{M} , indicated by $\dot{\nu}^\circ$ is given by

$$\dot{\nu}^\circ = \dot{\nu} + \mathcal{A}(\nu)q, \quad (7.2)$$

where

$$\mathcal{A}(\nu) = \frac{d\nu_{\phi(Q)}}{d\phi} \frac{d\phi(Q)}{dq} \Big|_{q=0}, \quad (7.3)$$

with $\nu_{\phi(Q)}$ the value of ν after the action of $\phi(Q) \in \text{Diff}(\mathcal{M}, \mathcal{M})$. Notice that each choice of ϕ defines an observer change. The previous formula takes into account that every element of $SO(3)$ can be expressed in the form $Q = \exp(q \times)$, with $q \in \mathbb{R}^3$.

In rule (7.2) we do not have a translation-type effect because $\nu = \tilde{\nu}(x, t)$ describes the inner structure of a material element. A rigid translation of a reference frame in the whole physical space $\tilde{\mathbb{R}}^3$ does not alter the way an observer records a microstructure at y . The case of rotations can be different, unless ν is a scalar or a pseudo-scalar, a circumstance that requires a special treatment, as we will see in the sequel.

We can think of a second class of observer changes, one also affecting the reference space \mathbb{R}^3 .

Let $w := \tilde{w}(x) \in \mathbb{R}^3$ be the value of a vector field over \mathcal{B} recorded by \mathcal{O} and w' the corresponding value measured by another observer \mathcal{O}' differing by \mathcal{O} in terms of a rigid-body motion. The counterpart of \dot{y}° , indicated here by w° , is given by

$$w^\circ = w + \bar{c} + \bar{q} \times (x - x_0), \quad (7.4)$$

where \bar{c} and \bar{q} are the values of smooth vector functions depending only on time.

More general classes of observer changes can be defined by considering the action of generic diffeomorphisms on both $\tilde{\mathbb{R}}^3$ and \mathbb{R}^3 . Their sets are indicated by $\text{Diff}(\tilde{\mathbb{R}}^3, \tilde{\mathbb{R}}^3)$ and $\text{Diff}(\mathbb{R}^3, \mathbb{R}^3)$, respectively. The infinitesimal generator of their action are vector fields over $\tilde{\mathbb{R}}^3$ and \mathbb{R}^3 , with values $v \in \tilde{\mathbb{R}}^3$ and $w \in \mathbb{R}^3$. Under observer changes determined by elements of $\text{Diff}(\tilde{\mathbb{R}}^3, \tilde{\mathbb{R}}^3)$, \dot{y}° assumes a more general structure indicated by \dot{y}° and given by

$$\dot{y}^\circ = \dot{y} + \tilde{v} . \quad (7.5)$$

Evidently, $\dot{y}^\circ = \dot{y}^\circ$ when $\tilde{v} = c + q \times (y - y_0)$. The family of differentiable homeomorphisms \mathcal{F} extends and becomes $\tilde{\mathcal{F}} := \{\tilde{\phi} : \text{Diff}(\tilde{\mathbb{R}}^3, \tilde{\mathbb{R}}^3) \rightarrow \text{Diff}(\mathcal{M}, \mathcal{M})\}$. We have $\mathcal{F} \subset \tilde{\mathcal{F}}$. Thus, \dot{v}° changes into \dot{v}° given by

$$\dot{v}^\circ = \dot{v} + \bar{v} , \quad (7.6)$$

where \bar{v} is the value of a tangent field to \mathcal{M} . Precisely, with $\alpha \mapsto \hat{\phi}_\alpha \in \tilde{\mathcal{F}}$ a differentiable curve over $\tilde{\mathcal{F}}$, we have $\dot{v}^\circ = \left. \frac{d\hat{\phi}_\alpha}{d\alpha} \right|_{\alpha=0}$. Moreover, w° changes into w° and involves a generic vector field:

$$w^\circ = w + \bar{w} . \quad (7.7)$$

8. Power and invariance

Actions are defined by the power they perform in every *conceptually* independent mechanism described by the time rate of entities representing the body morphology.

(a) External power

First, we refer to the *external power*, the one performed by agencies *external* to a generic body part $\mathfrak{b} \subseteq \mathcal{B}$. It is indicated by $\mathcal{P}_\mathfrak{b}^{ext}$ and defined by

$$\mathcal{P}_\mathfrak{b}^{ext}(\dot{y}, \dot{v}) := \int_\mathfrak{b} (b^\dagger \cdot \dot{y} + \beta^\dagger \cdot \dot{v}) dx + \int_{\partial\mathfrak{b}} (t_\partial \cdot \dot{y} + \tau_\partial \cdot \dot{v}) d\mathcal{H}^2(x) . \quad (8.1)$$

In the previous formula, $b^\dagger := \tilde{b}^\dagger(x, t)$ and $t_\partial := \tilde{t}_\partial(x, t)$ are body forces and traction already described in §3; $\beta^\dagger := \tilde{\beta}^\dagger(s, t)$ is the counterpart of b^\dagger and represents bulk actions directly affecting the microstructure (for example an electromagnetic action on molecules undergoing polarization). It is assumed to be the sum of inertial, β^{in} , and non-inertial, β , contributions, namely $\beta^\dagger = \beta^{in} + \beta$; $\tau_\partial := \tilde{\tau}_\partial(x, t)$ is a contact interaction between first-neighbour microstructures, owing to relative rearrangement of one with respect to the other, it depends on space, time and the boundary $\partial\mathfrak{b}$. In geometrical terms, $\tilde{b}^\dagger(x, t)$ and $\tilde{t}_\partial(x, t)$ belong to $T_x^*\mathcal{B}$, while $\tilde{\beta}^\dagger(s, t)$ and $\tilde{\tau}_\partial(x, t)$ to $T_{\tilde{v}(x, t)}^*\mathcal{M}$.

We define $\mathcal{P}_\mathfrak{b}^{ext}(\dot{y}, 0)$ as the external power of standard actions; $\mathcal{P}_\mathfrak{b}^{ext}(0, \dot{v})$ is the external power of microstructural actions. We require invariance of $\mathcal{P}_\mathfrak{b}^{ext}(\dot{y}, \dot{v})$ under isometry-based observer changes, namely we impose

$$\mathcal{P}_\mathfrak{b}^{ext}(\dot{y}, \dot{v}) = \mathcal{P}_\mathfrak{b}^{ext}(\dot{y}^\circ, \dot{v}^\circ) , \quad (8.2)$$

for any choice of \mathfrak{b} and the vectors c, q appearing in rules (7.1) and (7.2). In other words, equation (8.2) is a requirement of objectivity for the external power. The arbitrariness of c implies the integral balances of forces. The arbitrariness of q implies a non-standard balance of couples (or moments), which includes the projection over $\tilde{\mathbb{R}}^3$ of the microstructural actions β^\dagger and τ_∂ through \mathcal{A}^* , the formal adjoint of \mathcal{A} . Standard boundedness and regularity assumptions on the integral balance of forces imply by Cauchy's theorem 2.1 the representation of t_∂ in terms of first Piola–Kirchhoff's stress; C^1 -regularity grants the local balance of forces. Analogous assumptions imply from the non-standard integral balance of couples the representation of τ_∂

in terms of a stress tensor—called a *microstress*—and the existence of a *self-action*, indicated by z ; both contribute to balance β^{\ddagger} when C^1 -regularity occurs so that we have the *local balance of microstructural interactions*. Also, microstress and self-action make non-symmetric Cauchy's stress with symmetry-breaking terms that are of order $O(\lambda^2)$ —recall that λ is the spatial scale ν refers to. The whole procedure is a special case of what is described in the next section, so we postpone details. Here, we only recall that, beyond the evolution of microstructures, the balance of microstructural actions can describe even the evolution of defects in three different ways:

- (1) ν can be chosen to represent directly defects at a spatial scale λ ; for example, ν can represent damage (be it isotropic or anisotropic), the dislocation density tensor in crystalline structures, the plastic factor F^p in Kröner–Lee's multiplicative decomposition $F = F^e F^p$, its curl that represents Burgers' tensor, the slip time rate in a single crystal, etc.
- (2) ν is not directly related to a description of a defect, meaning it describes another generic microstructural feature as for example the local direction of molecular alignment in liquid crystals, but its singularities accounts for nucleation and/or evolution of defects at scale λ . In equilibrium conditions, the nucleation of such defects may emerge as a consequence of topological obstructions to energy relaxation [55,56].
- (3) ν can be chosen to be the indicator function of a macroscopic defect although the balance equations can furnish solutions taking values in the interval $[0,1]$ rather than in the set $\{0,1\}$; what the equations foresee is thus a sort of mushy transition region [57]. This scalar choice implies a problem that we discuss below.

There is also another problem: the requirement of invariance for the external power does not cover nucleation and/or evolution of defects *at a scale greater than λ* in a body endowed *per se* with (active) microstructure, the geometric features of which, not necessarily associated with a defect, are described by ν . The basic reason is that the procedure adopted above assumes that the reference configuration is fixed once and for all while, in the presence of evolving macroscopic defects, it is appropriate to consider virtually varying (said also *parameterized* or *mutant*, as already recalled) reference configurations.

A new concept is useful to analyse this situation on the basis of invariance requirements. Such a concept is the one of the so-called *relative power*.

(b) Relative power

Consider an evolving macroscopic bulk defect in the current configuration \mathcal{B}_c . It implies at least a local loss of one-to-one correspondence between \mathcal{B}_c and \mathcal{B} assured by \tilde{y} in the absence of defect evolution. When such an evolution occurs, at t , the current configuration $\mathcal{B}_c := \tilde{y}(\mathcal{B}, t)$ is in one-to-one correspondence with a reference configuration that differs from \mathcal{B} only by the identification of a subset that is the immaterial image of the defect in \mathcal{B}_c (roughly speaking a 'shadow'). We may thus consider *a family of infinitely many reference configurations* that differ from one another only by subsets that are virtual loci corresponding to which a defect is in \mathcal{B}_c . However, instead of considering the whole family of possible reference configurations, we may refer to an *infinitesimal generator* of it, a differentiable vector field

$$x \longmapsto w := \tilde{w}(x) \in \mathbb{R}^3. \quad (8.3)$$

Thus, we have three kinematically independent mechanisms: those described by \dot{y} , $\dot{\nu}$ and w . This idea is a version of the way Eshelby [58] and Gurtin [59] in independent works considered mutant (that is, virtually varying) reference configurations, strictly mimicking the idea of (so-called) horizontal variations in calculus of variations (see, e.g. [56]).

To account for the additional mechanism represented by w , we need to write a power that is relative to w and reduces to $\mathcal{P}_b^{\text{ext}}(\dot{y}, \dot{\nu})$ when $w = 0$. We call it a *relative power* and write for it $\mathcal{P}_b^{\text{rel}}(\dot{y}, \dot{\nu}, w)$. Its definition takes into account that nucleation and growth of macroscopic defects induce inhomogeneity in the energy distribution with production of fluxes,

and rupture/reformation of material bonds with pertinent driving forces. We thus consider a free energy density ψ , taken to be a differentiable function of space, time and a list ζ of state variables *left unspecified* at this stage. We also consider a driving force field with values $f \in T_x^* \mathcal{B}$ at x and t , which is not related to a potential. It is a *configurational* action in the terminology introduced by Nabarro [60]. Finally, we include a configurational couple with values $\bar{\mu} \in T_x^* \mathcal{B}$ at x and t . For a generic body part $\mathfrak{b} \subseteq \mathcal{B}$ that is free of low-dimensional defects with own surface or line energy, but possibly including a bulk defect, the *relative power*, introduced in [61], and refined in [62,63], is defined by

$$\mathcal{P}_{\mathfrak{b}}^{rel}(\dot{y}, \dot{v}, w) := \mathcal{P}_{\mathfrak{b}}^{rel-a}(\dot{y}, \dot{v}, w) + \mathcal{P}_{\mathfrak{b}}^{dis}(w), \quad (8.4)$$

with

$$\begin{aligned} \mathcal{P}_{\mathfrak{b}}^{rel-a}(\dot{y}, \dot{v}, w) := & \int_{\mathfrak{b}} (b^\dagger \cdot (\dot{y} - Fw) + \beta^\dagger \cdot (\dot{v} - Nw)) \, dx \\ & + \int_{\partial \mathfrak{b}} (t_0 \cdot (\dot{y} - Fw) + \tau_0 \cdot (\dot{v} - Nw)) \, d\mathcal{H}^2(x) \end{aligned} \quad (8.5)$$

the *relative power of actions* and

$$\mathcal{P}_{\mathfrak{b}}^{dis}(w) := \int_{\partial \mathfrak{b}} (n \cdot w) \psi \, d\mathcal{H}^2(x) - \int_{\mathfrak{b}} (\partial_x \psi + f) \cdot w \, dx + \int_{\mathfrak{b}} \bar{\mu} \cdot \text{curl} w \, dx, \quad (8.6)$$

a *power of disarrangement*. In the previous expression, $\partial_x \psi$ is the explicit derivative of ψ with respect to x , holding fixed the state variables in the list ζ , that is $\partial_x \psi := \left. \frac{\partial \psi(x, t, \zeta)}{\partial x} \right|_{\zeta \text{ fixed}}$.

We require objectivity for $\mathcal{P}_{\mathfrak{b}}^{rel}$. Thus, we impose

$$\mathcal{P}_{\mathfrak{b}}^{rel}(\dot{y}, \dot{v}, w) = \mathcal{P}_{\mathfrak{b}}^{rel}(\dot{y}^\circ, \dot{v}^\circ, w^\circ), \quad (8.7)$$

for any choice of c, q, \bar{c}, \bar{q} appearing in rules (7.1), (7.2), (7.4) and \mathfrak{b} . The linearity of $\mathcal{P}_{\mathfrak{b}}^{rel}$ implies

$$\mathcal{P}_{\mathfrak{b}}^{rel}(c + q \times (y - y_0), \mathcal{A}(v)q, \bar{c} + \bar{q} \times (x - x_0)) = 0. \quad (8.8)$$

The arbitrariness of c, q, \bar{c} and \bar{q} implies, respectively, the integral balance of standard forces,

$$\int_{\mathfrak{b}} b^\dagger \, dx + \int_{\partial \mathfrak{b}} t_0 \, d\mathcal{H}^2(x) = 0, \quad (8.9)$$

a non-standard integral balance of couples already mentioned in the previous section,

$$\int_{\mathfrak{b}} ((y - y_0) \times b^\dagger + \mathcal{A}^* \beta^\dagger) \, dx + \int_{\partial \mathfrak{b}} ((y - y_0) \times t_0 + \mathcal{A}^* \tau_0) \, d\mathcal{H}^2(x) = 0, \quad (8.10)$$

a balance of configurational actions,

$$\int_{\partial \mathfrak{b}} (\psi In - F^* t_0 - N^* \tau_0) \, d\mathcal{H}^2(x) - \int_{\mathfrak{b}} (F^* b^\dagger + N^* \beta^\dagger) \, dx - \int_{\mathfrak{b}} (\partial_x \psi + f) \, dx = 0, \quad (8.11)$$

and an integral balance of configurational couples,

$$\begin{aligned} \int_{\partial \mathfrak{b}} (x - x_0) \times (\psi In - F^* t_0 - N^* \tau_0) \, d\mathcal{H}^2(x) - \int_{\mathfrak{b}} (x - x_0) \times (F^* b^\dagger + N^* \beta^\dagger) \, dx \\ - \int_{\mathfrak{b}} (x - x_0) \times (\partial_x \psi + f) \, dx - \int_{\mathfrak{b}} 2e(\bar{\mu} \times) \, dx = 0. \end{aligned} \quad (8.12)$$

When $|b^\dagger|$ is bounded over \mathcal{B} and t_0 is continuous over \mathcal{B} , Cauchy's theorem 2.1 implies $t_0 = t := \tilde{t}(x, t, n)$ at all points of $\partial \mathfrak{b}$ where the normal n is well defined, with $\tilde{t}(x, t, n) = -\tilde{t}(x, t, -n)$, and $t := \tilde{t}(x, t, n) = P(x, t)n$, with $P(x, t) \in \text{Hom}(T_x^* \mathcal{B}, T_{\tilde{y}(x, t)}^* \mathcal{B}_c)$ the first Piola–Kirchhoff stress tensor already mentioned in §3. Thus, if for every t the map $x \mapsto P(x)$ is $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$, with

$\bar{\mathfrak{b}}$ the closure of the reference configuration, and $x \mapsto b^\dagger$ is continuous, the arbitrariness of \mathfrak{b} implies from equation (8.9) the standard pointwise balance

$$b^\dagger + \text{Div}P = 0. \quad (8.13)$$

Set $\mathbf{r} := (y - y_0) \times b^\dagger + \mathcal{A}^* \beta^\dagger$ and $\mathbf{s}_\partial := (y - y_0) \times t + \mathcal{A}^* \tau_\partial$. The integral balance (equation (8.10)) reads

$$\int_{\mathfrak{b}} \mathbf{r} \, dx + \int_{\partial \mathfrak{b}} \mathbf{s}_\partial \, d\mathcal{H}^2(x) = 0. \quad (8.14)$$

Since \mathcal{B} is bounded, we can choose y_0 in a way such that the boundedness of $|b^\dagger|$ implies the one of $|(y - y_0) \times b^\dagger|$. When, in addition, $|\mathcal{A}^* \beta^\dagger|$ is also bounded over \mathcal{B} and τ_∂ is continuous with respect to x , by Cauchy's theorem we obtain $\mathbf{s}_\partial = \tilde{\mathbf{s}}(x, t, n) = -\tilde{\mathbf{s}}(x, t, -n)$ at all points of $\partial \mathfrak{b}$ where the normal n is well defined. Thus, since $\tilde{\mathbf{s}}(x, t, n) = (y - y_0) \times \tilde{\tau}(x, t, n) + \mathcal{A}^* \tau_\partial$, we have $\tau_\partial = \tau := \tilde{\tau}(x, t, n)$ and, since $\tilde{\tau}(x, t, n) = -\tilde{\tau}(x, t, -n)$,

$$\mathcal{A}^*(\tilde{\tau}(x, t, n) + \tilde{\tau}(x, t, -n)) = 0. \quad (8.15)$$

This means that only the projection on the physical space of τ satisfies the action–reaction principle; the principle may be satisfied on \mathcal{M} only when 0 belongs to the kernel of \mathcal{A}^* , the formal adjoint of \mathcal{A} . In addition, $\tilde{\mathbf{s}}(x, t, n)$ is linear with respect to n : there exist $\mathfrak{H}(x, t) \in \text{Hom}(T_x^* \mathcal{B}, T_{\tilde{y}(x, t)}^* \mathcal{B}_c)$ such that $\tilde{\mathbf{s}}(x, t, n) = \mathfrak{H}(x, t)n$; thus

$$\mathfrak{H}(x, t)n = (y - y_0) \times P(x, t)n + \mathcal{A}^* \tilde{\tau}(x, t, n). \quad (8.16)$$

Consequently, there exists $S(x, t) \in \text{Hom}(T_x^* \mathcal{B}, T_{\tilde{y}(x, t)}^* \mathcal{M})$ such that

$$\tilde{\tau}(x, t, n) = S(x, t)n. \quad (8.17)$$

In proving the existence of the microstress S we do not embed \mathcal{M} into any linear space, unlike what has been proposed in [64], where such an embedding is adopted. Since \mathcal{M} is finite-dimensional, by Whitney's theorem an embedding of \mathcal{M} into a linear space always exists; it can be even isometric, owing to Nash's theorems, but it is not unique and the dimension of the target space depends on the regularity of the embedding. Avoiding it grants an intrinsic character to the theory.

With these results, when in addition to P even the microstress S is $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$, the integral balance (equation (8.10)) becomes

$$\int_{\mathfrak{b}} ((y - y_0) \times b^\dagger + \mathcal{A}^* \beta^\dagger) \, dx + \int_{\mathfrak{b}} ((y - y_0) \times \text{Div}P - ePF^* + \mathcal{A}^* \text{Div}S + (DA^*)^t S) \, dx = 0, \quad (8.18)$$

where e is Ricci's alternating index and the superscript t means minor right transposition for third-rank tensors. When bulk terms are continuous, the arbitrariness of $\mathfrak{b} \subseteq \mathcal{B}$ implies that, pointwise in \mathcal{B} ,

$$-ePF^* + \mathcal{A}^*(\beta^\dagger + \text{Div}S) + (DA^*)^t S = 0. \quad (8.19)$$

Since $\beta^\dagger \in T_{\tilde{y}}^* \mathcal{M}$ and also $\text{Div}S \in T_{\tilde{y}}^* \mathcal{M}$, we can read equation (8.19) by saying that there exists $z \in T_{\tilde{y}}^* \mathcal{M}$ such that

$$\text{skw}PF^* = \frac{1}{2}e(\mathcal{A}^*z + (DA^*)^t S), \quad (8.20)$$

and

$$\beta^\dagger - z + \text{Div}S = 0. \quad (8.21)$$

This last relation is the *balance of microstructural actions*. Equation (8.20) states that in this setting the standard Cauchy stress $\sigma = \frac{1}{\det F}PF^*$ is generally non-symmetric. It is symmetric

when $e(\mathcal{A}^*z + (D\mathcal{A}^*)^t S) = 0$ when we neglect terms of the order λ^2 , with λ , we recall, the spatial scale ν refers to (see proof in [65]).

With these results, equation (8.11) reads

$$\int_{\partial\mathfrak{b}} (\psi I - F^*P - N^*S)n \, d\mathcal{H}^2(x) - \int_{\mathfrak{b}} (F^*b^\dagger + N^*\beta^\dagger) \, dx - \int_{\mathfrak{b}} (\partial_x\psi + f) \, dx = 0. \quad (8.22)$$

Thus, by setting $\mathbb{P} := \psi I - F^*P - N^*S$ and considering the assumed continuity of the bulk terms, the arbitrariness of \mathfrak{b} implies the *local balance of configurational actions* in \mathcal{B} :

$$\text{Div}\mathbb{P} - F^*b^\dagger - N^*\beta^\dagger - \partial_x\psi = f. \quad (8.23)$$

Also, equation (8.10) becomes

$$\int_{\partial\mathfrak{b}} (x - x_0) \times \mathbb{P}n \, d\mathcal{H}^2(x) - \int_{\mathfrak{b}} (x - x_0) \times (F^*b^\dagger + N^*\beta^\dagger - \partial_x\psi - f) \, dx - \int_{\mathfrak{b}} 2\bar{\mu} \, dx = 0. \quad (8.24)$$

Consequently, under previous regularity conditions, and presuming that $\partial_x\psi$, f , and $\bar{\mu}$ are continuous, use of Gauss' theorem, validity of the local balance (equation (8.23)), and arbitrariness of \mathfrak{b} imply

$$\text{skw}(\mathfrak{g}^{-1}\mathbb{P}) = -\bar{\mu} \times. \quad (8.25)$$

The second-rank tensor \mathbb{P} is the appropriate version in the present setting of the *Hamilton–Eshelby's stress*, also called *Eshelby's stress*.

Cauchy's theorem 2.1 suggests also that the continuity assumptions concerning surface-dependent densities of boundary integrals in the previous sections can be weakened. Continuity has been adopted in this section only for the sake of simplicity.

The local balance equations above derived imply the identity

$$\mathcal{P}_{\mathfrak{b}}^{\text{rel}}(\dot{y}, \dot{\nu}, w) = \int_{\mathfrak{b}} (P \cdot \dot{F} + z \cdot \dot{\nu} + S \cdot \dot{N} + \text{sym}\mathbb{P} \cdot \text{sym}Dw) \, dx. \quad (8.26)$$

When $w = 0$, $\mathcal{P}_{\mathfrak{b}}^{\text{rel}}$ reduces to $\mathcal{P}_{\mathfrak{b}}^{\text{ext}}$ and we have

$$\mathcal{P}_{\mathfrak{b}}^{\text{ext}}(\dot{y}, \dot{\nu}) = \int_{\mathfrak{b}} (P \cdot \dot{F} + z \cdot \dot{\nu} + S \cdot \dot{N}) \, dx =: \mathcal{P}_{\mathfrak{b}}^{\text{int}}(\dot{y}, \dot{\nu}). \quad (8.27)$$

The last integral, namely $\mathcal{P}_{\mathfrak{b}}^{\text{int}}(\dot{y}, \dot{\nu})$, is what we call the *internal power*.

(c) Comparison with other approaches and limits of the invariance procedure

Balance of microstructural actions have been postulated in *local* (e.g. [36,40,47,66,67]), *integral* (e.g. [40, pp. 317–318], [30,68,69]) or *weak* form (e.g. [70,71]), or derived from a variational principle (e.g. [41,72]). The weak form is what we usually call a *principle of virtual power*; when we assume it as a first principle, as in [70], we need to postulate the expressions of both external and internal powers. The structure of the latter presumes existence of standard and microstructural stresses, and the self-action z , without deriving them from more fundamental structures.

Postulating integral balances allows one to get stresses as derived entities, rather than assuming their existence. There are also conditions, determined by Antman & Osborn [73], under which integral balances and the virtual power principle can be put into correspondence without adopting the necessary regularity for pointwise balances. However, postulating a general integral balance of microstructural actions can be questionable. Indeed, the maps associating with every $x \in \mathcal{B}$ the microstructural actions β^\dagger , z and Sn take values into $T^*\mathcal{M}$, which is a nonlinear space, unless \mathcal{M} itself is a linear space, which is *not* the generic case. So, integrals of microstructural actions are in general not defined. Also, as shown above, even when

\mathcal{M} is a linear space, postulating the integral balance of microstructural actions is superabundant if not superfluous.

Adopting a variational principle in conservative setting or a d'Alembert-type one, when certain dissipative effects occur, to derive balance equations implies putting on the same conceptual ground the derivation of balance equations and the prescription of constitutive structures, although they are at different conceptual levels [12]. In addition, a d'Alembert-type principle implies postulating existence of the stress, independently of the energy, when a dissipation pseudo-potential is not available.

Configurational balances have been also postulated [59] or derived from a variational principle [58].

In the path followed in the previous section, we *derive* balance equations of standard, microstructural and configurational actions from invariance of the relative power alone under appropriate classes of observer changes [62,63,74]. The need of a self-action z appears as a consequence of ν insensitivity to rigid translations of reference frames in the physical space. We avoid postulating the inner power.

The invariance procedure discussed here, however, fails when ν is a scalar or a pseudo-scalar because in these two cases $\mathcal{A} = 0$. We thus need something more. We discuss this issue below, after writing down an appropriate version of the Clausius–Duhem inequality.

9. Possible microstructural inertia

Microstructures might have at least in some cases relative inertia with respect to the overall body. Two examples are (i) a solid body with scattered small cavities including gyroscopes, each undergoing its own rotation, (ii) macro-molecules scattered in a ground fluids that may vibrate relatively to the fluid.

A general suggestion [47,75,76] is to consider the *kinetic energy* $\text{kin}(\mathfrak{b}; \dot{y}, \dot{\nu})$ of a generic body part $\mathfrak{b} \subseteq \mathcal{B}$ to be given by the sum

$$\text{kin}(\mathfrak{b}; \dot{y}, \dot{\nu}) := \int_{\mathfrak{b}} \left(\frac{1}{2} \rho |\dot{y}|^2 + \mathfrak{k}(\nu, \dot{\nu}) \right) dx, \quad (9.1)$$

where $\mathfrak{k}(\nu, \dot{\nu})$ is the *microstructural kinetic energy*, with $\mathfrak{k} : T^*\mathcal{B} \rightarrow \mathbb{R}$ a map assumed to be such that $\mathfrak{k}(\nu, 0) = 0$ and $\partial_{\dot{\nu}}^2 \mathfrak{k} \cdot (\dot{\nu} \otimes \dot{\nu}) \geq 0$, where the last identity holds if and only if $\dot{\nu} = 0$. We assume that

$$\frac{d}{dt} \text{kin}(\mathfrak{b}; \dot{y}, \dot{\nu}) = - \int_{\mathfrak{B}} (b^{in} \cdot \dot{y} + \beta^{in} \cdot \dot{\nu}) dx \quad (9.2)$$

for any choice of the velocity fields. Arbitrariness of \dot{y} implies

$$b^{in} = -\rho \dot{y}^{\flat}, \quad (9.3)$$

where \dot{y}^{\flat} is the covector naturally associated with the acceleration \ddot{y} by a spatial metric. So, the integral balance (equation (9.2)) reduces to

$$\frac{d}{dt} \int_{\mathfrak{B}} \mathfrak{k}(\nu, \dot{\nu}) dx = - \int_{\mathfrak{B}} \beta^{in} \cdot \dot{\nu}_{rel} dx. \quad (9.4)$$

We thus consider [47,75] a function $\chi(\nu, \dot{\nu})$ such that

$$\mathfrak{k}(\nu, \dot{\nu}) = \frac{\partial \chi(\nu, \dot{\nu})}{\partial \dot{\nu}} \cdot \dot{\nu} - \chi(\nu, \dot{\nu}). \quad (9.5)$$

Consequently, the arbitrariness of $\dot{\nu}$ implies

$$\beta^{in} = \frac{\partial \chi}{\partial \nu} - \frac{d}{dt} \frac{\partial \chi}{\partial \dot{\nu}}. \quad (9.6)$$

A problem, however, may occur. Consider $\mathfrak{k}(\nu, \dot{\nu})$ to be such that

$$\mathfrak{k}(\nu, \dot{\nu}) = \frac{1}{2}(\Xi \dot{\nu}) \cdot \dot{\nu}, \quad (9.7)$$

with $\Xi \in \text{Hom}(T_\nu \mathcal{M}, T_\nu^* \mathcal{M})$ a positive-definite second-rank tensor. Take a rigid motion with macroscopic velocity $\dot{y}_r(x, t) := c(t) + q(t) \times (y - y_0)$ and phase field time rate $\dot{\nu}_r(x, t) = \mathcal{A}(\nu)q$ (in both expressions the subscript r means *rigid-type*). We compute

$$\text{kin}(\mathfrak{b}; \dot{y}, \dot{\xi}) := \frac{1}{2}q \cdot \left(\widehat{\mathfrak{I}} + \int_{\mathfrak{b}} \frac{1}{2} \mathcal{A}^* \Xi \mathcal{A} \, dx \right) q, \quad (9.8)$$

where $\widehat{\mathfrak{I}}$ is the standard inertia tensor. So, accounting for the microstructure would increase the inertial tensor $\widehat{\mathfrak{I}}$, which seems to be doubtful because the microstructure is internal to every material element. To avoid such a problem, we could consider \mathfrak{k} as a function of ν and $\dot{\nu}_{rel} := \dot{\nu} - \mathcal{A}q$, namely $\mathfrak{k} = \mathfrak{k}(\nu, \dot{\nu}_{rel})$. We thus take a function $\chi = \chi(\nu, \dot{\nu}_{rel})$ such that

$$\mathfrak{k}(\nu, \dot{\nu}_{rel}) = \frac{\partial \chi(\nu, \dot{\nu}_{rel})}{\partial \dot{\nu}_{rel}} \cdot \dot{\nu}_{rel} - \chi(\nu, \dot{\nu}_{rel}). \quad (9.9)$$

Then, with constant mass density ρ , we assume the inertial balance

$$\frac{d}{dt} \int_{\mathfrak{B}} \left(\frac{1}{2} \rho |\dot{y}|^2 + \mathfrak{k}(\nu, \dot{\nu}_{rel}) \right) dx + \int_{\mathfrak{B}} \frac{\partial \chi(\nu, \dot{\nu}_{rel})}{\partial \nu} \cdot \mathcal{A}q \, dx = - \int_{\mathfrak{B}} (b^{in} \cdot \dot{y} + \beta^{in} \cdot \dot{\nu}_{rel}) \, dx, \quad (9.10)$$

and presume that it holds for any choice of the velocity fields. Arbitrariness of \dot{y} implies once again $b^{in} = -\rho \ddot{y}$. The inertial balance (equation (9.10)) reduces to

$$\frac{d}{dt} \int_{\mathfrak{B}} \mathfrak{k}(\nu, \dot{\nu}_{rel}^b) \, dy + \int_{\mathfrak{B}} \frac{\partial \chi(\nu, \dot{\nu}_{rel})}{\partial \nu} \cdot \mathcal{A}q \, dx = - \int_{\mathfrak{B}} \beta^{in} \cdot \dot{\nu}_{rel} \, dx, \quad (9.11)$$

so, the time derivative of \mathfrak{k} , equation (9.9), and the arbitrariness of $\dot{\nu}_{rel}$ imply

$$\beta^{in} = \frac{\partial \chi}{\partial \nu} - \frac{d}{dt} \frac{\partial \chi}{\partial \dot{\nu}_{rel}}. \quad (9.12)$$

The proposal of considering $\dot{\nu}_{rel}$ in the kinetic energy needs further analyses.

10. Thermodynamics

(a) First law

Internal energy is an extensive entity represented by a Radon measure with a density e with respect to the volume measure. In particular, the internal energy density e is a differentiable state function. Write r for a (scalar) *heat source density*, and \bar{a}_δ for a (scalar) *heat flux* through the boundary $\partial \mathfrak{b}$. For every body part $\mathfrak{b} \subseteq \mathcal{B}$ the first law of thermodynamics reads

$$\frac{d}{dt} \int_{\mathfrak{b}} e \, dx - \mathcal{P}_{\mathfrak{b}}^{ext}(\dot{y}, \dot{\nu}) - \int_{\mathfrak{b}} r \, dx + \int_{\partial \mathfrak{b}} \bar{a}_\delta \, d\mathcal{H}^{k-1}(x) = 0, \quad (10.1)$$

for any choice of \mathfrak{b} and the velocity fields involved.

Assume that $\mathcal{P}_{\mathfrak{b}}^{ext}(\dot{y}, \dot{\nu})$ is bounded. In addition, presume also that \dot{e} and r are bounded, while \bar{a}_δ is continuous with respect to x . Cauchy's theorem 2.1 implies that \bar{a}_δ depends on $\partial \mathfrak{b}$ only through the normal n to $\partial \mathfrak{b}$ in all points where n is well-defined, namely $\hat{a}_\delta = \bar{a}(x, t, n)$, and

$$\bar{a}(x, t, n) = -\bar{a}(x, t, -n); \quad (10.2)$$

we find also existence of a vector field \tilde{q} depending only on x and t such that

$$\bar{a}(x, t, n) = \tilde{q}(x, t) \cdot n. \quad (10.3)$$

Then, thanks to the identity $\mathcal{P}_b^{ext}(\dot{y}, \dot{v}) = \mathcal{P}_b^{int}(\dot{y}, \dot{v})$, equation (10.1) becomes

$$\frac{d}{dt} \int_b e \, dx - \mathcal{P}_b^{int}(\dot{y}, \dot{v}) - \int_b r \, dx + \int_{\partial b} \tilde{q}(x, t) \cdot n \, d\mathcal{H}^{k-1}(x) = 0. \quad (10.4)$$

When \dot{e} , r , and \mathcal{P}_b^{int} are continuous with respect to x , and $\tilde{q}(\cdot, t)$ is $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$, the arbitrariness of b implies the local energy balance

$$\dot{e} - P \cdot \dot{F} - z \cdot \dot{v} - S \cdot \dot{N} - \hat{r} + \text{Div} \tilde{q} = 0. \quad (10.5)$$

(b) Second law

Entropy is also an extensive entity represented by a Radon measure. We write η for its density with respect to the volume measure and state the second law as follows:

$$\frac{d}{dt} \int_b \eta \, dx \geq \int_b \bar{s} \, dx - \int_{\partial b} \bar{h}_\partial \, d\mathcal{H}^{k-1}(x). \quad (10.6)$$

We assume that it holds for any choice of $b \subseteq \mathcal{B}$ and the rate fields involved. In the previous inequality, \bar{s} is the entropy source, and \bar{h}_∂ a (scalar) flux depending on ∂b in addition to x and t .

If $\dot{\eta}$ and \bar{s} are bounded, we can apply even in this case Cauchy's theorem 2.1: the key aspect in its proof is an estimate on the boundary integral; so we need only an inequality, not necessarily a balance. Then, if \bar{h}_∂ is continuous with respect to x , we find that it depends on ∂b only through the normal n at all points where n is well-defined. Thus, we have

$$\bar{h}_\partial(x, t) = \tilde{h}(x, t, n) = -\tilde{h}(x, t, -n), \quad (10.7)$$

and there is a vector field with values \bar{h} , depending only on x and t , such that

$$\tilde{h}(x, t, n) = \bar{h}(x, t) \cdot n. \quad (10.8)$$

If $\dot{\eta}$ and \bar{s} are continuous with respect to x , while \bar{h} is $C^1(\mathcal{B}) \cap C(\bar{\mathcal{B}})$, the arbitrariness of b implies

$$\dot{\eta} \geq \bar{s} - \text{Div} \bar{h}. \quad (10.9)$$

(c) The Clausius–Duhem inequality

Defining temperature beyond thermodynamic equilibrium is a debated issue. A possible view is to consider the absolute temperature as a label for states that links heat flux and source with their counterparts in the second law (see [6,77]). In this way, the absolute temperature ϑ is defined by the law it satisfies.

We thus consider the relations

$$\bar{s} = \frac{r}{\vartheta}, \quad \bar{h} = \frac{\tilde{q}}{\vartheta} + \varpi, \quad (10.10)$$

where ϖ is a *residual entropy flux* owing to microstructural effects. Precisely, we presume that

$$\varpi = \tilde{\varpi}(\nu, \dot{\nu}, D\nu, \vartheta, \dots), \quad (10.11)$$

where the dots indicate that the functional dependence can include all derivatives of the state variables considered, according to Truesdell's principle of equipresence. Explicit expressions for ϖ depend on specific cases considered. Equation (10.10) appeared first in [78] with no explicit reference to microstructures.

Thus, with ψ the Helmholtz free energy density defined to be $\psi := e - \vartheta\eta$, we have

$$\dot{\psi} + \dot{\eta} - P \cdot \dot{F} - z \cdot \dot{\nu} - S \cdot \dot{N} + \frac{1}{\vartheta} \tilde{q} \cdot D\vartheta - \vartheta \text{Div} \varpi \leq 0. \quad (10.12)$$

It is a version of the *Clausius–Duhem inequality*, presumed to hold for *any choice* of the rate fields involved. After Coleman's & Noll's 1959 work [79], we commonly consider the inequality as a source of constitutive restrictions and admissibility criteria. However, this is not the sole role that can be acquired by the second law. In any case, maintaining here the traditional viewpoint, we presume that

$$\{\psi, \eta, P, z, S\}(F, \nu, N, \vartheta; \dot{F}, \dot{\nu}, \dot{N}, \dot{\vartheta}), \quad (10.13)$$

meaning with the previous notation that all entities in the first parentheses depend on the state variables listed on the right-hand side. In particular, ψ is assumed to be differentiable with respect to its entries. We compute $\dot{\psi} = \frac{\partial \psi}{\partial F} \cdot \dot{F} + \frac{\partial \psi}{\partial \nu} \cdot \dot{\nu} + \frac{\partial \psi}{\partial N} \cdot \dot{N} + \frac{\partial \psi}{\partial \vartheta} \dot{\vartheta} + \frac{\partial \psi}{\partial \dot{F}} \cdot \dot{F} + \frac{\partial \psi}{\partial \dot{\nu}} \cdot \dot{\nu} + \frac{\partial \psi}{\partial \dot{N}} \cdot \dot{N} + \frac{\partial \psi}{\partial \dot{\vartheta}} \dot{\vartheta}$. By inserting the result in relation (10.12), the arbitrariness of all rate fields involved implies necessarily that $\psi = \tilde{\psi}(F, \nu, N, \vartheta)$, so that the dissipation inequality reduces to

$$\frac{\partial \psi}{\partial F} \cdot \dot{F} + \frac{\partial \psi}{\partial \nu} \cdot \dot{\nu} + \frac{\partial \psi}{\partial N} \cdot \dot{N} + \frac{\partial \psi}{\partial \vartheta} \dot{\vartheta} - P \cdot \dot{F} - z \cdot \dot{\nu} - S \cdot \dot{N} + \frac{1}{\vartheta} \tilde{q} \cdot D\vartheta - \vartheta \text{Div} \varpi \leq 0. \quad (10.14)$$

We consider for P , z and S an additive decomposition into energetic (meaning determined by ψ) and dissipative components, respectively indicated by the superscripts (e) and (d):

$$P = P^{(e)} + P^{(d)} = \tilde{P}^{(e)}(F, \nu, N, \vartheta) + \tilde{P}^{(d)}(F, \nu, N, \vartheta; \dot{F}, \dot{\nu}, \dot{N}, \dot{\vartheta}), \quad (10.15)$$

$$z = z^{(e)} + z^{(d)} = \tilde{z}^{(e)}(F, \nu, N, \vartheta) + \tilde{z}^{(d)}(F, \nu, N, \vartheta; \dot{F}, \dot{\nu}, \dot{N}, \dot{\vartheta}), \quad (10.16)$$

$$S = S^{(e)} + S^{(d)} = \tilde{S}^{(e)}(F, \nu, N, \vartheta) + \tilde{S}^{(d)}(F, \nu, N, \vartheta; \dot{F}, \dot{\nu}, \dot{N}, \dot{\vartheta}), \quad (10.17)$$

while, for the entropy density, we have $\eta = \tilde{\eta}(F, \nu, N, \vartheta)$, which means that we refer to equilibrium entropy, the non-equilibrium production being assigned to the term $\vartheta \text{Div} \varpi$. Thus, we have

$$\begin{aligned} & \left(\frac{\partial \psi}{\partial F} - P^{(e)} \right) \cdot \dot{F} + \left(\frac{\partial \psi}{\partial \nu} - z^{(e)} \right) \cdot \dot{\nu} + \left(\frac{\partial \psi}{\partial N} - S^{(e)} \right) \cdot \dot{N} + \left(\frac{\partial \psi}{\partial \vartheta} + \eta \right) \dot{\vartheta} \\ & - P^{(d)} \cdot \dot{F} - z^{(d)} \cdot \dot{\nu} - S^{(d)} \cdot \dot{N} + \frac{1}{\vartheta} \tilde{q} \cdot D\vartheta - \vartheta \text{Div} \varpi \leq 0. \end{aligned} \quad (10.18)$$

The arbitrariness of time rates involved implies

$$P^{(e)} = \frac{\partial \psi}{\partial F}, \quad z^{(e)} = \frac{\partial \psi}{\partial \nu}, \quad S^{(e)} = \frac{\partial \psi}{\partial N}, \quad (10.19)$$

and the local dissipation inequality

$$P^{(d)} \cdot \dot{F} + z^{(d)} \cdot \dot{\nu} + S^{(d)} \cdot \dot{N} - \frac{1}{\vartheta} \tilde{q} \cdot D\vartheta + \vartheta \text{Div} \varpi \geq 0. \quad (10.20)$$

Specific choices for $P^{(d)}$, $z^{(d)}$ and $S^{(d)}$ must be compatible with this last inequality.

(d) Equilibrium states in the elastic case

Consider the energy density $e(x, F)$ of elastic simple bodies. The physical incompatibility between the convexity of e with respect to F and its objectivity imposes that e be at least polyconvex with respect to F , that is, a lower semicontinuous convex function of all minors of F , that is of F itself, $\text{cof} F$ and $\det F$. Ball's [80] existence theorem on minimizing deformation in $W^{1,p}$, $p > 3$, requires that $e(x, F) \geq c_1(|F|^2 + |\text{cof} F|^2) + f(\det F)$, with $f(\cdot)$ a function growing to infinity when $\det F$ goes to zero. With respect to $W^{1,p}$, a refinement by Müller *et al.* [81] includes the case $p = 3$. Below such an exponent, deformations in $W^{1,p}$ may display discontinuities

such as cavitation and fractures. Also, neo-Hookean materials, which do not satisfy the above boundedness form below, may have dipole-like singularities [82]. To avoid such problems, we need an additional condition that allows a selection in $W^{1,p}$ of a suitable subspace of maps that can describe appropriately what we commonly intend as elastic behaviour of simple bodies. We find naturally such conditions when we look at deformations in terms of Cartesian currents, so that we can select a subspace of $W^{1,p}$, $p > 1$, of so-called *weak diffeomorphism*, as introduced in [83] (see also [56]).

If we forget strain and consider only an elastic energy of the type $e(x, \nu, D\nu)$, when ν is a unit vector (so, \mathcal{M} is the unit sphere S^2), even in the simplest case in which $e = \frac{1}{2}|D\nu|^2$, minimizers may display the formation of topological defects (specifically point and line charges, and dipoles; see [55,56,84]) under Dirichlet-type boundary conditions. The question is open when the energy density e is non-convex with respect to $D\nu$ because lower semicontinuity results for manifold-valued maps are not available when the manifold is not embedded into a linear space.

When we look at \mathcal{M} maintaining it as generic as possible and look at complex bodies with energy density $\tilde{e}(x, F, \nu, D\nu)$, existence theorems of energy minimizers are available under different specific assumptions about \mathcal{M} , the map $x \mapsto \nu$, and the structure of e [85–87].

There is, however, something more beyond the conservative setting.

(e) Covariance of the second law

As already mentioned, when ν is a scalar or a pseudo-scalar, the linear operator $\mathcal{A}(\nu)$ appearing in the equation (7.2) vanishes. Thus, the procedure based on a requirement of objectivity for the external power or the relative one does not allow one to deduce a *scalar* balance of microstructural interactions. Indeed, such a scalar balance has been postulated (e.g. in [30,69]). However, even in this case something more fundamental can be done. We can require covariance of the Clausius–Duhem inequality, written in an appropriate way. Covariance means here structure invariance under diffeomorphism-based observer changes given by relations (7.5), (7.6) and (7.7). This approach does not necessarily require that ν is a scalar or a pseudo-scalar. It holds for ν in a generic \mathcal{M} , including scalar and pseudo-scalar cases. Also, this approach includes as special cases the requirements of objectivity for the external power and the relative one. It has been formulated in a general way in [65] and anticipated to an extent in [88,89].

The following axiom is at its roots: *if a phenomenon does not produce energy for a given observer, any other observer differing from the first one by diffeomorphisms must record the same property.*

In other words, the axiom states that the conservative or dissipative character of a phenomenon is intrinsic, meaning observer independent. For the sake of simplicity, we write down here only an isothermal version of the Clausius–Duhem inequality for a generic body part that is free of low-dimensional defects endowed with their own surface or line energies, but possibly including a bulk defect. Thus, the inequality reads as

$$\int_{\mathfrak{b}} \dot{\psi} \, dx - \mathcal{P}_{\mathfrak{b}}^{\text{rel}}(\dot{y}, \dot{v}, w) \leq 0. \quad (10.21)$$

By imposing the covariance axiom to the inequality (10.21), we must prescribe rules of how the time rate of the free energy ψ varies under diffeomorphism-based observer changes because ψ is a density associated with the volume measure, and diffeomorphism generically alter the volume unless they are chosen to be volume-preserving. A general rule proposed in [65] for the time rate of the free energy reads as

$$\dot{\psi} \mapsto \dot{\psi}^\circ = \dot{\psi} + \varphi(\zeta; \nabla \bar{v}, \bar{v}, \nabla \bar{v}, \bar{w}, \nabla \bar{w}, \dots), \quad (10.22)$$

where the last addendum is an arbitrary smooth function depending on the state ζ , which is *left unspecified*, while the other terms are the infinitesimal generators of the actions of the diffeomorphism group on the physical space, the reference one and the manifold \mathcal{M} , together with their

derivatives. The function φ is assumed to be Galilean invariant in the physical space and to vanish under isometry-based observer changes. Here just observable entities are accounted for. The presence of non-observable entities, however, cannot be excluded, depending on specific modelling choices. Consequences of the axiom are thus (i) the representation of contact actions in terms of stresses, (ii) the action–reaction principle, (iii) the existence of a microstructural self-action, (iv) the local balance of standard and microstructural actions, the latter ones even in the case of scalar (or pseudo-scalar) phase fields, (v) the local balance of configurational actions, (vi) constitutive restrictions, (vii) admissibility criteria (at times adding a maximum dissipation principle). In this path, dissipation is obviously included. All above ‘entities’ emerge from the role of observers, that is, from a requirement of structural invariance of the second law under different observations. Extending the result to non-isothermal setting is rather straightforward. Proofs are in [65]. The results give a new role to the second law, with respect to its standard use. Put simply, *every basic structure of a continuum model comes from the covariance requirement for the second law of thermodynamics written as an appropriate form of the Clausius–Duhem inequality.*

11. Special internal constraints on the phase field and further topics

(a) Strain gradient elasticity and Korteweg’s fluids

Consider an elastic complex body with energy $e := \tilde{e}(x, F, \nu, N)$. Assume also that there is an internal constraint

$$\nu = \hat{\nu}(F), \quad (11.1)$$

with $\hat{\nu}$ a differentiable \mathcal{M} -valued function. An immediate consequence is that $\tilde{e}(x, F, \nu, N) = \tilde{f}(x, F, DF)$. The interaction measures admit an additive decomposition into active and reactive components, indicated, respectively, by the superscripts a and r . So, we have $P = P^{(a)} + P^{(r)}$, $z = z^{(a)} + z^{(r)}$, and $S = S^{(a)} + S^{(r)}$. The reactive components are assumed to be powerless. This means that they are such that

$$P^{(r)} \cdot \dot{F} + z^{(r)} \cdot \dot{\nu} + S^{(r)} \cdot \dot{N} = 0. \quad (11.2)$$

Since $\dot{\nu} = \frac{\partial \nu}{\partial F} \dot{F}^*$, by substituting into [condition \(11.2\)](#), we find an expression of the stress P that is free of the reactive components, and a third-rank hyperstress with components given by

$$\left(\frac{\partial \nu^\alpha}{\partial F} \right)_i^A S_\alpha^B, \quad (11.3)$$

where the Greek index indicates coordinates over \mathcal{M} , lower case indices refer to the physical space, while upper case ones indicate components in the reference space, and summation over repeated indices is adopted. Strain-gradient elasticity thus emerges; the balance of microstructural interactions is embedded into the standard pointwise balance of forces: itself the microstructure becomes *latent* in the terminology introduced by Capriz [66]. Following this view, we do not need to prove existence of the third-rank hyperstress *per se*, rather, the existence proof of the microstress S is sufficient to get the resulting hyperstress with [components \(11.3\)](#).

When we reduce the internal [constraint \(11.1\)](#) to $\nu = \det F$ and refer to balance equations in Eulerian form, we recover Korteweg’s fluids [66].

(b) Influence of microstructural variations on temperature propagation

Neglect macroscopic strain, while allowing microstructure to vary in time. Can we say that this behaviour is the one of a *rigid body with microstructure*? The answer depends on what we consider to be a rigid body. An appropriate definition is that a body is rigid when it admits only

isometries as possible deformations. So, we can speak of a rigid body with microstructure when ν does not affect the strain measures. Presume in addition that $\beta^{\ddagger} = 0$, so that $\text{Div}S = z$. Thus, under these restricted conditions $P = 0$ and $z \cdot \dot{\nu} + S \cdot \dot{N} = \text{Div}(S^*\dot{\nu})$. Write p for the covector $S^*\dot{\nu}$, so that the local energy balance reduces to

$$\dot{e} - \hat{r} + \text{Div}(\tilde{q} - p) = 0. \quad (11.4)$$

Assume that ν depends on temperature, that is

$$\nu = \bar{\nu}(\vartheta), \quad (11.5)$$

with $\bar{\nu}$ a differentiable \mathcal{M} -valued function (a physically significant case is the one of strontium–titanate that undergoes temperature-dependent polarization; for such material ν is the polarization vector). Under the internal constraint (11.5), the energy $e = \tilde{e}(\vartheta, \nu, N)$ becomes $e = \hat{e}(\vartheta, D\vartheta)$ (notice that F is absent because we are in a condition under which at most $F = R \in SO(3)$). Thus, by taking Fourier's law $\tilde{q} = -\kappa D\vartheta$ and $p = \hat{p}(\vartheta, D\vartheta, \vartheta)$, with \hat{p} assumed to be differentiable with respect to its entries, the reduced local energy balance (equation (11.4)) becomes

$$\left(\frac{\partial e}{\partial D\vartheta} - \frac{\partial p}{\partial \vartheta} \right) \cdot D\dot{\vartheta} + \frac{\partial e}{\partial \vartheta} \dot{\vartheta} - \kappa \Delta \vartheta - \frac{\partial p}{\partial \vartheta} \cdot D\vartheta - \frac{\partial p}{\partial D\vartheta} \cdot D^2\vartheta - r = 0 \quad (11.6)$$

(see also [90]). Consider $\frac{\partial p}{\partial D\vartheta}$ to be negligible and look at one-dimensional setting. In this case, equation (11.6) reduces to

$$\zeta_{\vartheta} \frac{\partial^2 \vartheta}{\partial t \partial x} + c_v \frac{\partial \vartheta}{\partial t} - \kappa \frac{\partial^2 \vartheta}{\partial x^2} + \xi_{\vartheta} \frac{\partial \vartheta}{\partial x} - r = 0, \quad (11.7)$$

where $\zeta_{\vartheta} := \frac{\partial e}{\partial D\vartheta} - \frac{\partial p}{\partial \vartheta}$, $c_v := \frac{\partial e}{\partial \vartheta}$ and $\xi_{\vartheta} := -\frac{\partial p}{\partial \vartheta}$. Equation (11.7) is hyperbolic. It avoids the paradox of infinite speed temperature propagation as determined by the balance of energy in rigid conductors when p is absent. As a special case, assume that the coefficients in equation (11.7) are constant. Travelling waves $\vartheta(x, t) = u(x - ct)$ are admissible with velocities c given by

$$c = -\frac{\kappa}{\zeta}, \quad c = \frac{\xi}{c_v}, \quad c = \frac{\xi - \kappa\alpha}{\zeta\alpha + c_v}, \quad (11.8)$$

where α is a constant that appears in an initial condition of the type $\bar{a}_1 \exp(\alpha x) + \bar{a}_2 x + \bar{a}_3$, where $\bar{a}_1, \bar{a}_2, \bar{a}_3$ are constant, and $\alpha \neq 0$, $\alpha \neq -\frac{c_v}{\zeta}$ [91].

(c) Another possible view on non-parabolic heat propagation

Consider the case in which the dissipative components of standard stress and microstress, namely $P^{(d)}$ and $S^{(d)}$, vanish in the inequality (10.20), and $z^{(d)}$ is intrinsically dissipative, meaning that it satisfies the inequality $z^{(d)} \cdot \dot{\nu} \geq 0$ for any $\dot{\nu}$, the identity holding only when $\dot{\nu} = 0$. The remaining dissipation inequality $-\frac{1}{\vartheta} \tilde{q} \cdot D\vartheta + \vartheta \text{Div} \varpi \geq 0$ is compatible with $\tilde{q} = -\kappa D\vartheta + q$, where q is a non-Fourier component of the heat flux such that $q \cdot D\vartheta = \vartheta^2 \text{Div} \varpi$. Assume $\nu = q$, meaning that we consider the non-Fourier component as determined by the microstructure at a scale λ . Under further special constitutive assumptions, to within λ^2 terms, the balance of microstructural interactions in Eulerian form reduces to Guyer–Krumhansl's equation, while the local energy balance to Payne–Song's equation (the proof is in [63]). These two equations are essential to evaluate stability of non-isothermal flows (see analyses in [92,93]), and can be used to describe fluids with pollutants [94].

(d) Further topics

There are several other topics connected with what is presented here. They would deserve to be reported and discussed widely but this would extend this article beyond the limits imposed. One of these topics is the evolution of structured interfaces in complex media; they are characterized by a possibly non-constant surface energy. Beyond Cauchy's or Piola–Kirchhoff's type surface stress, largely analysed in the common setting of continuum mechanics, in the case of complex media we have occurrence of a *surface* microstress and a *surface* microstructural self-actions. Besides significant special cases (e.g. nematic–isotropic interfaces in liquid crystals [95], solidification of two-phase fluids [96]), a general theory of surface microstructural interactions is available [97] and suggests further analyses in the general model-building setting.

Another topic is the analysis of microstructural influence on crack propagation. Indeed, ν can be chosen as the indicator function of a crack path (phase-field modelling of fracture, see, e.g. [57]). However, we can refer to cases of a fracture in an already complex material described in the multi-field setting sketched above. There are non-trivial effects of microstructural influences on cracks in special cases (see, e.g. [44,98–100]); general views are also available [101,102], and open the way to further analyses.

Data accessibility. This article has no additional data.

Declaration of AI use. I have not used AI-assisted technologies in creating this article.

Authors' contributions. P.M.M.: conceptualization, formal analysis, investigation, methodology, supervision, writing—original draft, writing—review and editing.

Conflict of interest declaration. I declare I have no competing interests.

Funding. The support of GNFM-INDAM is acknowledged.

Acknowledgements. This paper is largely based on personal notes written for a PhD course delivered online from the University of Florence in 2021. I thank Jaime Planas for several discussions on the topics tackled in the course. I also thank the reviewers and the Editor for their analyses. This work belongs to activities of the research group 'Theoretical Mechanics' in the 'Centro di Ricerca Matematica Ennio De Giorgi', part of the Scuola Normale Superiore Pisa. GNFM-INDAM is also acknowledged.

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