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Continuum kinematics with incompatible–compatible decomposition

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We present a framework for the kinematics of a material body undergoing anelastic deformation. For such processes, the material structure of the body, as reflected by the geometric structure given to the set of body points, changes. The setting we propose may be relevant to phenomena such as plasticity, fracture, discontinuities and non-injectivity of the deformations. In this framework, we construct an unambiguous decomposition into incompatible and compatible factors that includes the standard elastic–plastic decomposition in plasticity.

This article is part of the theme issue 'Foundational issues, analysis and geometry in continuum mechanics'.

1. Introduction

The elastic–plastic decomposition of the deformation gradient, F, into an 'elastic' factor, F^e, and a 'plastic' factor, F^p, as $F = F^e F^p$, was introduced in 1960 by Kröner [1] and in 1967 by Lee & Liu [2,3], and has been used and studied extensively since then. For a comprehensive review of the subsequent work, see [4], and for more recent work see for example [5–13]. The plastic factor is viewed as the tensor field needed in order to release the residual stresses in the reference unloaded configuration of the body. The incompatibility reflects the macroscopic description of the existence of defects in the material. From another point of view, e.g. [12–14], it is impossible to embed isometrically the body with the stress-free metric tensor in a three-dimensional Euclidean space. Under such interpretations, the elastic factor, F^e, describes the incompatible packing of the stress-free body elements to restore compatibility to $F = F^e F^p$.

Another view on the elastic–plastic decomposition is proposed by Reina & Conti [15–17] where starting from a perfect lattice, F^p corresponds to a change of material structure of the lattice—a change in the topology—while F^e corresponds to the placement of the defected structure in space.

The following exemplifies some approaches to motivate the elastic–plastic decomposition.

— By looking at lattices and considering a notion of defectiveness defined referring to invariant peculiar features with respect to the action of diffeomorphisms, G. Parry arrived at a multiplicative decomposition that involves two factors of the type F^p, one preceding F^e, the other following it [18].
— In crystals, slips may occur along special planes and are a source of unrecoverable strain determined by the slip of dislocations. Across such planes, deformations suffer jumps of finite amplitude. A way to model the circumstance is selecting deformations to be special maps of bounded variations (SBV-maps). Such maps admit a distributional derivative that is a measure with an additive decomposition into a bulk part, which is absolutely continuous with respect to the Lebesgue volume measure, and a singular component concentrated over a rectifiable set with $m-1$ Hausdorff dimension, where m is the dimension of the domain. The multiplicative decomposition $F = F^e F^p$ emerges naturally, as shown by Reina & Conti [15] (see also [16,17,19]; the latter reference accounts for possible volumetric plastic changes in the SBV setting). In this view, F^p is a measure, while F^e a gradient, taken with positive determinant. In [16] the plastic deformation is shown to follow from a coarse-graining procedure from the lattice mesoscopic description.

Here, we propose a framework that shares similarities with these last two approaches. Like [16], we view the plastic factor as assignment of topological structure to the body. Similarly to [18], we take material structure to be invariant under a subgroup of the group of diffeomorphisms.

When we refer to continuum mechanics, we commonly say that it is the qualitative and quantitative description of the way tangible bodies react under external actions. The definition requires clarification of the essential nature of what we call a *body*: this is a conceptual choice, we need to make—and we do this even unconsciously—in building up mathematical models of natural phenomena.

In basic treatises on continuum mechanics—mainly those emerging from the work of C. A. Truesdell's school—a body is taken to be a set of not otherwise specified *material elements*, presumed to be endowed with the structure of a finite-dimensional manifold [20–25]. In particular, in [20], the manifold structure of body is manifested by its configurations in the three-dimensional Euclidean space.

This setting may be extended to the situation where the physical space is modelled as a general n-dimensional manifold, $\mathscr{S}$. Such a generalization may be motivated, for example, by considering small scale interactions, or microstructure. In this case, configurations will be valued in a fibre bundle over a Euclidean space [26–29].

Anelasticity is associated with changes of material structure—the topological or geometric structure of the material body. Thus, one has to make a clear distinction between a body, which has a certain manifold structure, and the collection of points that the body comprises. To identify the object, the material structure of which may change in an anelastic process, we use the term *protobody*. The various material structures that a protobody may attain in anelastic processes are

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referred to as *embodiments*. Each embodiment of a protobody should be a body of continuum mechanics. (See [30,31], where analogous notions are presented for theories of growing bodies.)

The configuration space, $\mathscr{Q}$, of a protobody in space, should contain all the configurations in space at all possible embodiments of the body. To each configuration κ of the protobody in space, there corresponds an embodiment e of the protobody. However, it is expected that for each embodiment there will be a subset of configurations of the protobody.

Thus, we say that two configurations, κ_1 and κ_2, of the protobody correspond to the same embodiment if there is a diffeomorphism, g_{21}, of the space manifold such that $\kappa_2 = g_{21} \circ \kappa_1$. This induces an equivalence relation on $\mathscr{Q}$, for which an embodiment is an equivalence class, and the embodiment space, $\mathscr{E}$, is the quotient set.

Next, we show that an embodiment, e, may be represented as a topological space, $\mathscr{B}_e$, the elements of which are the body points associated with that embodiment. It is noted that we do not restrict configurations of the protobody to be injective. As a result, the topological spaces $\mathscr{B}_{e_1}$ and $\mathscr{B}_{e_2}$, for two distinct embeddings need not comprise the same material points. Finally, each configuration $\kappa : \mathscr{B} \to \mathscr{S}$ is factored in the form $\kappa = \kappa_e \circ \kappa_{ae}$, where $\kappa_{ae} : \mathscr{B} \to \mathscr{B}_e$ and $\kappa_e : \mathscr{B}_e \to \mathscr{S}$, the analogue of the elastic–plastic decomposition. There is no ambiguity in the decomposition.

This general framework makes it possible to represent discontinuous and non-injective configurations of the protobody in space, modelling phenomena such as fracture and destruction of material points.

To consider phenomena such as plasticity for which the elastic–plastic decomposition applies to the deformation gradient, we have to be more specific. Thus, we substitute for the protobody the tangent bundle $T\mathscr{B}$ of a manifold $\mathscr{B}$, representing the perfect crystallographic structure of the body. A configuration is represented by a vector bundle morphism $\kappa : T\mathscr{B} \to T\mathscr{S}$. Incompatibility occurs when κ is not the tangent mapping of the base map $\underline{\kappa} : \mathscr{B} \to \mathscr{S}$. We say that two configurations, κ_1 and κ_2, correspond to the same embodiment when there is a diffeomorphism, g_{21}, of space such that $\kappa_2 = Tg_{21} \circ \kappa_1$. We show that an embodiment is represented by a vector bundle, representing the 'dislocated' material structure, and the elastic–plastic decomposition of vector bundle configurations of a protobody follows.

Section 2 outlines the general framework we propose for the kinematics of elastic-anelastic processes. Section 3 describes some of the notions of the general framework in terms of groupoids. This section may be skipped without interrupting the rest of the text. Section 4 considers the case where configurations are vector bundle morphisms defined on the tangent bundle of a manifold. As mentioned above, the tangent bundle represents a solid body together with its microstructure. Section 5 specializes the foregoing one to the case where the base mapping of the vector bundle morphisms representing the configurations, are embeddings. This situation is analogous, in the geometry of differentiable manifolds, to the classical elastic–plastic decomposition described above. Finally, in §6, we make some comments as to the relevance of the proposed framework to quasi-crystals.

2. The basic framework

(a) Basic definitions

Let $\mathscr{B}$ be a set, which we view as a collection of material points, and refer to it as a *protobody*. We do not assume at this stage that $\mathscr{B}$ has any particular structure. As a standard example, the protobody may be represented by a bounded open subset of $\mathbb{R}^3$.

The *physical space* is modelled by an n-dimensional oriented differentiable manifold $\mathscr{S}$. In traditional formulations of continuum mechanics $\mathscr{S}$ is modelled as a three-dimensional Euclidean space.

The *configuration space*, $\mathscr{Q}$, of the protobody is assumed to be a given class of mappings of the protobody into the space manifold. A generic element of $\mathscr{Q}$ is denoted as $\kappa : \mathscr{B} \to \mathscr{S}$. For example, if $\mathscr{B}$ is a bounded and connected open subset of $\mathbb{R}^3$ and $\mathscr{S} = \mathbb{R}^3$, one may consider the case where $\mathscr{Q} = BV(\mathscr{B}, \mathbb{R}^3)$, or $\mathscr{Q} = \mathrm{SBV}^p(\mathscr{B}, \mathbb{R}^3)$, with appropriate p, when discontinuities of the deformation distributional derivative (a measure, indeed) do not include a Cantor set and the absolutely continuous part with respect to the Lebesgue measure is endowed with L^p density.

In the rest of the text, we refer to *bi-Lipschitz, oriented diffeomorphisms* simply as *diffeomorphisms*. On a differentiable manifold, bi-Lipschitz mappings may be defined using a Riemannian metric. The class of bi-Lipschitz mappings is invariant under the particular choice of a Riemannian metric.

Definition 2.1. Let G be a subgroup of the group of diffeomorphisms of $\mathscr{S}$. We say that $\kappa_1, \kappa_2 \in \mathscr{Q}$ are *compatible* if there is a diffeomorphism $g_{21} \in G$ such that

$$\kappa_2 = g_{21} \circ \kappa_1. \tag{2.1}$$

In such a case, we refer to g_{21} as a (compatible) *displacement* and we write $\kappa_1 \sim \kappa_2$.

Remark 2.2. As a possible generalization of this definition one may consider a group of bijective mappings $\mathscr{S} \to \mathscr{S}$ that are not necessarily smooth. This may lead to a relaxed definition of the compatible (elastic) factor of the decomposition. For example, one may consider a subgroup of the group of bi-Lipschitz mappings on $\mathscr{S}$.

Evidently, compatibility is an equivalence relation, which justifies the notation we adopt.

Definition 2.3. The quotient space,

$$\mathscr{E} := \mathscr{Q}/\sim \tag{2.2}$$

will be referred to as the *space of material structures* or the *embodiment space*. An element $e \in \mathscr{E}$ represents a *material structure* or an *embodiment*.

Thus, we have a natural projection

$$\pi_{\mathscr{E}} : \mathscr{Q} \longrightarrow \mathscr{E}, \qquad \kappa \longmapsto [\kappa], \tag{2.3}$$

where $[\kappa]$ denotes the equivalence class of κ.

(b) The structure induced by an embodiment

Any embodiment induces a topological space. In fact, let $e \in \mathscr{E}$ be an embodiment, and define

$$A_e := \coprod_{\kappa \in e} \text{Image}\,\kappa. \tag{2.4}$$

An element $a \in A_e$ is represented by (y, κ) where $y \in \text{Image}\,\kappa \subset \mathscr{S}$, $\kappa \in e$.

Consider the following relation on A_e. We say that

$$a_1 = (y_1, \kappa_1) \sim_e a_2 = (y_2, \kappa_2) \quad \text{if } y_2 = g_{21}(y_1) \tag{2.5}$$

for $g_{21} \in G$ satisfying $\kappa_2 = g_{21} \circ \kappa_1$. By the definition of $\mathscr{E}$, such a diffeomorphism exists. Evidently, $\sim_e$ is an equivalence relation. The equivalence class of $a \in A_e$ will be denoted as $[a]_e$. The quotient space $A_e/\sim_e$ will be denoted by $\mathscr{B}_e$, so that we have a natural projection

$$\pi_e : A_e \longrightarrow \mathscr{B}_e = A_e/\sim_e. \tag{2.6}$$

An element $x \in \mathscr{B}_e$ is interpreted as a *body point* contained in the embodiment e of the protobody. The set $\mathscr{B}_e$ is interpreted as the set of body points contained in the embodiment e. We may refer to $\mathscr{B}_e$ as the *body structure* induced by the embodiment e.

Let $e \in \mathscr{E}$ be an embodiment, and let $\kappa \in e$. We have a natural mapping

$$\pi_{e\kappa} : \text{Image}\,\kappa \longrightarrow \mathscr{B}_e, \quad y \longmapsto [(y, \kappa)]_e. \tag{2.7}$$

The mapping $\pi_{e\kappa}$ is clearly a bijection. The body point $x = \pi_{e\kappa}(y)$ occupies the location $y \in \mathscr{S}$ at the configuration κ.

Let $\kappa \in e$ be a configuration. Then, $\text{Image}\,\kappa$ has the subspace topology it inherits from the manifold $\mathscr{S}$. If $\kappa_1, \kappa_2 \in e$ so that $\kappa_2 = g_{21} \circ \kappa_1$, then, $g_{21}|_{\text{Image}\,\kappa_1} : \text{Image}\,\kappa_1 \to \text{Image}\,\kappa_2$ is a homeomorphism. This induces a topology on $\mathscr{B}_e$ by defining a subset $U \subset \mathscr{B}_e$ to be open if for some $\kappa \in e$, and an open subset $U_\kappa \subset \operatorname{Image}\kappa$,

$$U = \pi_{e\kappa}(U_\kappa). \tag{2.8}$$

The topology is well defined, and is independent of the choice of $\kappa \in e$. Moreover, with this topology, $\pi_{e\kappa} : \operatorname{Image}\kappa \to \mathscr{B}_e$ is a homeomorphism for each $\kappa \in e$.

In all practical cases, $\operatorname{Image}\kappa$ will be a topological submanifold of $\mathscr{S}$. If $\operatorname{Image}\kappa$ is an oriented differentiable submanifold of $\mathscr{S}$ for some $\kappa \in e$, this applies to all other $\kappa' \in e$. In this case, for $\kappa_1, \kappa_2 \in e$, $g_{21}|_{\operatorname{Image}\kappa_1} : \operatorname{Image}\kappa_1 \to \operatorname{Image}\kappa_2$ is a diffeomorphism. A procedure analogous to the one above induces an oriented manifold structure on $\mathscr{B}_e$ for which $\pi_{e\kappa}$ is a diffeomorphism.

(c) The incompatible–compatible decomposition

Let $\kappa : \mathscr{B} \to \mathscr{S}$ be a configuration, $\mathscr{I}_\kappa : \operatorname{Image}\kappa \to \mathscr{S}$ the natural inclusion, and $e = \pi(\kappa) \in \mathscr{E}$ the induced embodiment. Since $\pi_{e\kappa} : \operatorname{Image}\kappa \to \mathscr{B}_e$ is a homeomorphism, the same applies to $\pi_{e\kappa}^{-1}$ and we can define

$$\kappa_e := \mathscr{I}_\kappa \circ \pi_{e\kappa}^{-1} : \mathscr{B}_e \longrightarrow \mathscr{S}. \tag{2.9}$$

The mapping κ_e is interpreted as the *compatible factor of the configuration* κ. It is the analogue of the 'elastic' factor of the 'plastic-elastic' decomposition. Clearly, the compatible factor of the configuration is a continuous injection into $\mathscr{S}$. In case $\operatorname{Image}\kappa$ is an oriented submanifold of $\mathscr{S}$, and we use the induced differentiable structure on $\mathscr{B}_e$, κ_e is an embedding.

For the same variables as above, consider the mapping

$$\kappa_{ae} := \pi_{e\kappa} \circ \kappa : \mathscr{B} \longrightarrow \mathscr{B}_e. \tag{2.10}$$

Then,

$$\kappa = \kappa_e \circ \kappa_{ae}, \tag{2.11}$$

which is the incompatible–compatible decomposition (see the diagram below).

$$\begin{tikzcd}
 & \operatorname{Image}\kappa \subset \mathscr{S} \arrow[d, "\pi_{e\kappa}"'] \\
\mathscr{B} \arrow[ur, "\kappa"] \arrow[r, "\kappa_{ae}"'] & \mathscr{B}_e . \arrow[u, bend right, "\kappa_e"']
\end{tikzcd} \tag{2.12}$$

The relevance of the decomposition follows from the following property.

Lemma 2.4. *Let $\kappa \in Q$ be a configuration. Then, κ_{ae} depends only on $e = \pi_{\mathscr{E}}(\kappa) \in \mathscr{E}$.*

Proof. Let $X \in \mathscr{B}$ and $\kappa' \sim \kappa$. We have to show that $\kappa'_{ae}(X) = \kappa_{ae}(X)$. Since $\kappa' \sim \kappa$, there is a diffeomorphism, $g \in G$, such that $\kappa' = g \circ \kappa$. Hence, $\kappa'(X) = g(\kappa(X))$. By the definition (2.5),

$$(\kappa'(X), \kappa') \sim_e (\kappa(X), \kappa). \tag{2.13}$$

The definition of $\pi_{e\kappa}$ in (2.7), implies now that

$$\pi_{e\kappa'}(\kappa'(X)) = \pi_{e\kappa}(\kappa(X)). \tag{2.14}$$

■

When $\mathscr{B}$ has an oriented manifold structure, and κ is an oriented embedding, κ_{ae} is a diffeomorphism. Thus, in such a case, one can identify $\mathscr{B}$ with $\mathscr{B}_e$, i.e. κ_{ae} reduces to an identity. In general, $\mathscr{B}$ has no structure, and compatibility of $\kappa_{ae} : \mathscr{B} \to \mathscr{B}_e$ in the standard sense of continuum mechanics cannot even be defined. Intermediate situations, where the incompatibility of κ_{ae} is significant and well defined, are considered below.

(d) Reference configurations

A right inverse of $\pi_{\mathscr{E}}$,

$$r : \mathscr{E} \to \mathscr{Q}, \tag{2.15}$$

may be interpreted as a system of reference configurations for the embodiments of $\mathscr{B}$. In other words, $r(e)$ is the reference configuration for the material structure e in space.

When a system of reference configurations is given, one may accept the identification $\mathscr{B}_e :=$ Image $r(e)$. In such a situation, for some $\kappa \in \mathscr{Q}$, the deformation κ_e may be identified with the restriction,

$$g_{\kappa,r(e)}|_{\text{ Image } r(e)} : \text{ Image } r(e) \longrightarrow \mathscr{S}, \tag{2.16}$$

of the diffeomorphism $g_{\kappa,r(e)}$ of $\mathscr{S}$ to Image $r(e)$. The mapping κ_{ae} is identified in this case with $r(e)$. In case a system of reference configurations is not given, the term "intermediate' *configuration* does not describe the situation appropriately because κ_{ae} is valued in the abstract manifold $\mathscr{B}_e$ and not in space.

Also, although commonly used as a terminology in modelling plasticity, an 'intermediate' configuration intended as a *global* configuration obtained by rearranging in an incompatible way the material texture, is in general not available. In analysing strain, we essentially have a local description of the incompatibility due to the rearrangement of the material structure. We locally map the tangent space at a point in some configuration into an 'intermediate' space, and the mapping is incompatible in the sense of being not congruent. This circumstance leads us to model incompatibility of tangent-plane-neighbourhoods, as we do in §4.

3. The groupoid point of view

This section describes how some of the foregoing structure can be described and generalized using the language of groupoid theory. It is of a formal nature and may be skipped without interrupting the reading of the following sections. Roughly speaking, a groupoid consists of a collection of elements and a collection of arrows between pairs of elements. In particular, not all pairs of elements are connected by an arrow. Arrows can be composed and inverted in a consistent way.

In our situation, we have a set $\mathscr{Q}$, and a set Γ containing mappings. The configurations in $\mathscr{Q}$ are referred to as *objects* in the language of groupoid theory and the elements of Γ are referred to as *morphisms*. Each morphism, γ, is associated with a configuration $\kappa_1 = \alpha(\gamma)$ and a configuration $\kappa_2 = \beta(\gamma)$, and γ represents a mapping (a restriction of a diffeomorphism of $\mathscr{S}$ in the case considered above) Image $\kappa_1 \to$ Image κ_2. In such a case, we write $\kappa_2 = \gamma\kappa_1$.

The mappings $\alpha : \Gamma \to \mathscr{Q}$ and $\beta : \Gamma \to \mathscr{Q}$ are referred to as the *source map* and *target map*, respectively. Note that here, we do not require that the diffeomorphism be extended to a diffeomorphism of $\mathscr{S}$.

It is emphasized that not any pair of elements of $\mathscr{Q}$ are the source and target of some morphism. In general, there are pairs $\kappa_1, \kappa_2 \in \mathscr{Q}$, representing incompatible configurations of the body, for which there is no connecting morphism. For the case where there is a morphism γ such that $\kappa_2 = \gamma\kappa_1$, we have written $\kappa_2 \sim \kappa_1$.

The morphisms satisfy the following properties.

(i) α and β are surjective.

(ii) For *composable* morphisms $\gamma_1, \gamma_2 \in \Gamma$, that is $\beta(\gamma_1) = \alpha(\gamma_2)$, there is a composition $\gamma_2 \cdot \gamma_1 \in \Gamma$ such that

$$\alpha(\gamma_2 \cdot \gamma_1) = \alpha(\gamma_1) \quad \text{and} \quad \beta(\gamma_2 \cdot \gamma_1) = \beta(\gamma_2). \tag{3.1}$$

(iii) The composition is associative, so for three composable morphisms

$$\gamma_3 \cdot (\gamma_2 \cdot \gamma_1) = (\gamma_3 \cdot \gamma_2) \cdot \gamma_1. \tag{3.2}$$

(iv) For each $\kappa \in \mathscr{Q}$ there is a morphism ε_κ—corresponding to the identity mapping $\text{Image}\,\kappa \to \text{Image}\,\kappa$—such that $\alpha(\varepsilon_\kappa) = \beta(\varepsilon_\kappa) = \kappa$, and

$$\gamma \cdot \varepsilon_{\alpha(\gamma)} = \gamma = \varepsilon_{\beta(\gamma)} \cdot \gamma, \quad \text{for all} \quad \gamma \in \Gamma. \tag{3.3}$$

(v) For each $\gamma \in \Gamma$, there is $\gamma^{-1} \in \Gamma$, in our case the inverse mapping, such that

$$\gamma^{-1} \cdot \gamma = \varepsilon_{\alpha(\gamma)} \quad \text{and} \quad \gamma \cdot \gamma^{-1} = \varepsilon_{\beta(\gamma)}. \tag{3.4}$$

The restrictions of diffeomorphisms of $\mathscr{S}$, of the type $\text{Image}\,\kappa_1 \to \text{Image}\,\kappa_2$, evidently satisfy these conditions. This implies that Γ is a *groupoid* over $\mathscr{Q}$ and we express this as $\Gamma \rightrightarrows \mathscr{Q}$. (See [32] for the theory of groupoids and some of its applications to continuum mechanics.)

In the language of groupoid theory, the set

$$\mathscr{O}(\kappa) := \beta(\alpha^{-1}\{\kappa\}) = \alpha(\beta^{-1}\{\kappa\}) \subset \mathscr{Q} \tag{3.5}$$

is referred to as the *orbit* of κ. However, in our notation, the orbit is simply the equivalence class of κ—an embodiment of the body. The quotient space—the embodiment space in our application—is referred to as the *orbit space*.

Another groupoid structure corresponds to the construction of the set $\mathscr{B}_e$ for some given embodiment $e \in \mathscr{E}$. The space of objects in this case is A_e defined above, so that an object is represented by (y, κ), $y \in \text{Image}\,\kappa$. A morphism δ sends (y_1, κ_1) to (y_2, κ_2), where $\kappa_2 = \gamma\kappa_1$, $\gamma \in \Gamma$. Evidently, given κ_1 and κ_2, with $\kappa_2 = \gamma\kappa_1$, there is only a single $y_2 \in \text{Image}\,\kappa_2$ such that $(y_2, \kappa_2) = \delta(y_1, \kappa_1)$. The resulting groupoid will be denoted as $\Gamma_e \rightrightarrows A_e$. Thus, for the case described,

$$\alpha(\delta) = (y_1, \kappa_1) \quad \text{and} \quad \beta(\delta) = (y_2, \kappa_2). \tag{3.6}$$

Using the language of groupoids, a point $x \in \mathscr{B}_e$ is an orbit in Γ_e and $\mathscr{B}_e$ is the orbit space of Γ_e.

4. Infinitesimal incompatibility

For the case where $\mathscr{B}$ has an oriented manifold structure, a natural bundle morphism is associated with $\kappa : \mathscr{B} \to \mathscr{S}$; it is the tangent map, $T\kappa$, from $T\mathscr{B}$ to $T\mathscr{S}$. When we aim at describing elastic–plastic phenomena, we need to model incompatibility of tangent planes—'infinitesimal neighbourhoods' of material points—that may occur even in the case of smooth placements of the material points in space. To account for such incompatibility, we need to extend the view described so far. Specifically, we will no longer consider κ as a map from $\mathscr{B}$ to $\mathscr{S}$, rather, we take κ as a vector bundle morphism from $T\mathscr{B}$ to $T\mathscr{S}$.

(a) Infinitesimal configurations and embodiments

We specialize the setting of §2 by replacing first the protobody general set $\mathscr{B}$ by the tangent bundle, $T\mathscr{B}$ of an oriented manifold $\mathscr{B}$, where we have the projection

$$\tau_{\mathscr{B}} : T\mathscr{B} \longrightarrow \mathscr{B}. \tag{4.1}$$

The tangent space $T_X\mathscr{B}$ at $X \in \mathscr{B}$ represents the 'infinitesimal neighbourhood' of X.

The configuration space $\mathscr{Q}$ is a family of vector bundle morphisms

$$\kappa : T\mathscr{B} \longrightarrow T\mathscr{S}. \tag{4.2}$$

For $\kappa \in \mathscr{Q}$,

$$\underline{\kappa} : \mathscr{B} \longrightarrow \mathscr{S} \tag{4.3}$$

will denote the corresponding base map. It is assumed that $\underline{\kappa}$ is oriented. Incompatibility occurs when κ is not the tangent mapping $T\underline{\kappa}$ of some $\underline{\kappa} : \mathscr{B} \to \mathscr{S}$. It is assumed that for each $\kappa \in \mathscr{Q}$, Image κ is a subbundle of the restriction of $T\mathscr{S}$ to Image $\underline{\kappa}$. Thus, for each $\kappa \in \mathscr{Q}$, Image κ has a structure of a vector bundle with projection

$$\pi_\kappa : \text{ Image } \kappa \longrightarrow \text{ Image } \underline{\kappa}. \tag{4.4}$$

(Note that we use the notation κ for the vector bundle morphism rather than the traditional F in order to emphasize the analogy with the general case described above.)

Consider,

$$\underline{\mathscr{Q}} := \{\underline{\kappa} \mid \kappa \in \mathscr{Q}\}, \tag{4.5}$$

the set of all base mappings corresponding to the vector bundle morphisms in $\mathscr{Q}$. We have a natural projection

$$B : \mathscr{Q} \longrightarrow \underline{\mathscr{Q}} \qquad \kappa \longmapsto \underline{\kappa}. \tag{4.6}$$

The compatibility relation $\sim$ is now redefined as follows. The configurations κ_1 and κ_2 are compatible, that is, $\kappa_2 \sim \kappa_1$ if there exists some diffeomorphism, $g_{21} \in G$ of $\mathscr{S}$, the tangent map, $Tg_{21} : T\mathscr{S} \to T\mathscr{S}$, of which satisfies

$$\kappa_2 = Tg_{21} \circ \kappa_1. \tag{4.7}$$

Clearly, compatibility is an equivalence relation. Note that the collection, H, of mappings $T\mathscr{S} \to T\mathscr{S}$ that are of the form $h = Tg$, where g is a diffeomorphism of $\mathscr{S}$, is a subgroup of the group of all diffeomorphisms of $T\mathscr{S}$.

On $\underline{\mathscr{Q}}$ we can apply the construction described in §2, and define the equivalence relation

$$\underline{\kappa}_1 \underline{\sim} \underline{\kappa}_2 \quad \text{ if } \kappa_2 = g_{21} \circ \kappa_1, \tag{4.8}$$

for some $g_{21} \in G$. Evidently,

$$\underline{\kappa}_1 = B(\kappa_1) \underline{\sim} \underline{\kappa}_2 = B(\kappa_2), \quad \text{ if } \kappa_2 \sim \kappa_1. \tag{4.9}$$

The converse is false in general. For two distinct infinitesimal configurations such that the images of the base mappings are compatible, the infinitesimal structures need not be compatible. Once again we define the space of material structures, or the embodiment space, $\mathscr{E}$, to be the quotient space $\mathscr{Q}/\sim$, and we have the natural projection

$$\pi_{\mathscr{E}} : \mathscr{Q} \longrightarrow \mathscr{E} = \mathscr{Q}/\sim. \tag{4.10}$$

By our construction, the vector bundles of the form Image κ for the various elements $\kappa \in e \in \mathscr{E}$ are all vector bundle diffeomorphic. That is, if $\kappa_2 \sim \kappa_1$, then,

$$Tg_{21}|_{\text{Image } \kappa_1} : \text{ Image } \kappa_1 \longrightarrow \text{ Image } \kappa_2, \tag{4.11}$$

is a diffeomorphism of vector bundles.

In accordance with the previous section, we write

$$\underline{\pi}_{\underline{\mathscr{E}}} : \underline{\mathscr{Q}} \longrightarrow \underline{\mathscr{E}} := \underline{\mathscr{Q}}/\underline{\sim}, \tag{4.12}$$

for the natural projection induced by the equivalence relation $\underline{\sim}$.

Let $e \in \mathscr{E}$ be represented by κ, and let $\underline{e} = [\underline{\kappa} = B(\kappa)] \in \underline{\mathscr{E}}$. It follows from equation (4.9) that $\underline{e}$ is independent of the particular representative $\kappa \in e$. Hence, we have a surjection

$$B_\sim : \mathscr{E} \longrightarrow \underline{\mathscr{E}} \quad \text{ and } [\kappa] \longmapsto [B(\kappa)]. \tag{4.13}$$

Thus, $B_\sim^{-1}(\underline{e})$ is the collection of infinitesimal material structures for which the base material structure is $\underline{e}$.

(b) The structure corresponding to an infinitesimal embodiment

As in equation (2.4), A_e, $e \in \mathscr{E}$ is defined as the disjoint union of the images of all $\kappa \in e$. In analogy with (2.5), we define the equivalence relation $\sim_e$ in A_e by

$$a_1 = (v_1, \kappa_1) \sim_e a_2 = (v_2, \kappa_2) \quad \text{if } v_2 = Tg_{21}(v_1) \tag{4.14}$$

for $g_{21} \in G$ satisfying $\kappa_2 = Tg_{21} \circ \kappa_1$. In accordance with our notation scheme, we have

$$W_e := A_e/\sim_e \quad \text{and} \quad \pi_e : A_e \longrightarrow W_e. \tag{4.15}$$

Evidently, if $a_1 \sim_e a_2$, as above,

$$\pi_{\kappa_2}(v_2) = g_{21}(\pi_{\kappa_1}(v_1)). \tag{4.16}$$

Let $\underline{e} \in \underline{\mathscr{E}}$, and

$$\underline{A}_{\underline{e}} := \coprod_{\underline{\kappa} \in \underline{e}} \text{Image } \underline{\kappa}. \tag{4.17}$$

On $\underline{A}_{\underline{e}}$, we have the equivalence relation

$$\underline{a}_1 = (y_1, \underline{\kappa}_1) \simeq_{\underline{e}} \underline{a}_2 = (y_2, \underline{\kappa}_2) \quad \text{if } y_2 = g_{21}(y_1), \tag{4.18}$$

for some $g_{21} \in G$ satisfying $\underline{\kappa}_2 = g_{21} \circ \underline{\kappa}_1$. We set

$$\underline{\mathscr{B}}_{\underline{e}} = \underline{A}_{\underline{e}}/\simeq_{\underline{e}} \quad \text{and} \quad \underline{\pi}_{\underline{e}} : \underline{A}_{\underline{e}} \longrightarrow \underline{\mathscr{B}}_{\underline{e}}. \tag{4.19}$$

From (4.16) it follows that

$$(v_1, \kappa_1) \sim_e (v_2, \kappa_2) \quad \text{implies } (\pi_{\kappa_1}(v_1), \underline{\kappa}_1) \simeq_{\underline{e}} (\pi_{\kappa_2}(v_2), \underline{\kappa}_2). \tag{4.20}$$

We consider the quotient space, $W_e := A_e/\sim_e$, the structure of which is described below. We will show that W_e is a vector bundle over $\underline{\mathscr{B}}_{\underline{e}}$. The fibre over $x \in \underline{\mathscr{B}}_{\underline{e}}$ represents the infinitesimal material structure at x.

For $u = [(v, \kappa)]_e \in W_e$ ($[\cdot]_e$ indicates the equivalence class relative to $\sim_e$), we set

$$\pi_{W_e}(u) := [(\pi_\kappa(v), B(\kappa)]_{\underline{e}} = [(\pi_\kappa(v), \underline{\kappa}]_{\underline{e}} \in \underline{\mathscr{B}}_{\underline{e}}. \tag{4.21}$$

By (4.20), $\pi_{W_e}(u)$ is independent of the representative $(v, \kappa) \in A_e$, so we have a projection

$$\pi_{W_e} : W_e \longrightarrow \underline{\mathscr{B}}_{\underline{e}}. \tag{4.22}$$

Let $e \in \mathscr{E}$ be an embodiment, and let $\kappa \in e$. We have a natural mapping

$$\pi_{e\kappa} : \text{ Image } \kappa \longrightarrow W_e, \quad \text{and } v \longmapsto [(v, \kappa)]_e. \tag{4.23}$$

The mapping $\pi_{e\kappa}$ is a vector bundle diffeomorphism.

Similarly, let $\underline{e} \in \underline{\mathscr{E}}$, and let $\underline{\kappa} \in \underline{e}$. We have a natural diffeomorphism,

$$\underline{\pi}_{\underline{e\kappa}} : \text{ Image } \underline{\kappa} \longrightarrow \underline{\mathscr{B}}_{\underline{e}}, \quad y \longmapsto [(y, \underline{\kappa})]_{\underline{e}} \tag{4.24}$$

as in the previous section.

The induced decomposition is

$$\underline{\kappa} = \underline{\kappa}_{\underline{e}} \circ \underline{\kappa}_{\underline{ae}} \quad \text{and} \quad \underline{\kappa}_{\underline{e}} := \mathscr{I}_{\underline{\kappa}} \circ \underline{\pi}_{\underline{e\kappa}}^{-1} \tag{4.25}$$

and

$$\kappa = \kappa_e \circ \kappa_{ae}, \quad \kappa_{ae} := \pi_{e\kappa} \circ \kappa \quad \text{and} \quad \kappa_e := \mathscr{I}_\kappa \circ \pi_{e\kappa}^{-1}. \tag{4.26}$$

In fact, $\pi_{W_e} : W_e \longrightarrow \mathscr{B}_{\underline{e}}$ is a vector bundle that is the pullback of π_κ : Image $\kappa \to$ Image $\underline{\kappa}$ by $\underline{\kappa}_{\underline{e}}$. The resulting structure is illustrated in the following commutative diagram.

$$\begin{tikzcd}
 & & \mathrm{Image}\,\kappa \subset T\mathscr{S} \arrow[dl, "\pi_{e\kappa}"'] \arrow[dd, "\xi_\kappa"] \\
T\mathscr{B} \arrow[urr, "\kappa"] \arrow[r, "\kappa_{ae}"'] \arrow[dd, "\tau_{\mathscr{B}}"'] & W_e \arrow[ur, bend right, "\kappa_e"'] \arrow[dd, "\pi_{W_e}"] & \\
 & & \mathrm{Image}\,\underline{\kappa} \subset \mathscr{S} \arrow[dl, "\pi_{\underline{e\kappa}}"'] \\
\mathscr{B} \arrow[urr, "\underline{\kappa}"] \arrow[r, "\kappa_{\underline{ae}}"'] & \mathscr{B}_{\underline{e}} \arrow[ur, bend right, "\kappa_{\underline{e}}"'] &
\end{tikzcd} \tag{4.27}$$

In case a system of reference configurations $r : \mathscr{E} \to T\mathscr{S}$, a right inverse of $\pi_{\mathscr{E}}$ is given, the comments made in §2d, still apply. Looking at the decomposition $\kappa = \kappa_e \circ \kappa_{ae}$, we recover the standard multiplicative decomposition of the deformation gradient F, namely $F = F^e F^p$.

5. Deformations of dislocated crystals

The description of dislocated (periodic) crystals falls within the scheme built up so far. As above, the space manifold, $\mathscr{S}$, is an oriented n-dimensional manifold and the protobody $T\mathscr{B}$ is the tangent bundle of an oriented, compact, n-dimensional manifold with boundary. A configuration $\kappa \in \mathscr{Q}$ is assumed once again to be a vector bundle morphism

$$\kappa : T\mathscr{B} \longrightarrow T\mathscr{S}, \tag{5.1}$$

such that the base mapping, $\underline{\kappa} : \mathscr{B} \to \mathscr{S}$, is an oriented embedding, and for each $X \in \mathscr{B}$,

$$\kappa|_{T_X\mathscr{B}} : T_X\mathscr{B} \longrightarrow T_X\mathscr{S} \tag{5.2}$$

is an orientation preserving isomorphism.

The tangent bundle, $T\mathscr{B}$, is viewed as the perfect crystal lattice. Specifically, as a possible interpretation we can say that $\mathscr{B}$ is the set of atoms, itself the lattice structure, while considering $T\mathscr{B}$ allows us to assign at each point the pertinent optical axes. See also [33] where frames at the various material points represent the crystalline structure. The fact that κ need not be $T\underline{\kappa}$ reflects the dislocated configuration.

We set $\kappa_1 \sim \kappa_2$ if there is a diffeomorphism $g_{21} : \mathscr{S} \to \mathscr{S}$ such that $\kappa_2 = Tg_{21} \circ \kappa_1$. Evidently, if $\kappa_1 \sim \kappa_2 = Tg_{21} \circ \kappa_1$, then, $\underline{\kappa}_1 \simeq \underline{\kappa}_2$. Here, again, the equivalence relation $\underline{\kappa}_1 \simeq \underline{\kappa}_2$ is defined by the requirement that there is some diffeomorphism g_{21} of $\mathscr{S}$, such that $\underline{\kappa}_2 = g_{21} \circ \underline{\kappa}_1$. The spaces $\mathscr{E}$ and $\underline{\mathscr{E}}$ are defined in the previous section.

Let $\kappa_1, \kappa_2 \in \mathscr{Q}$ be arbitrary (not necessarily related). Then, since both $\underline{\kappa}_1$ and $\underline{\kappa}_2$ are embeddings, letting $\underline{\kappa}_1^{-1}$: Image $\underline{\kappa}_1 \to \mathscr{B}$ be the right inverse, we have a diffeomorphism

$$\underline{\kappa}_2 \circ \underline{\kappa}_1^{-1} : \mathrm{Image}\,\underline{\kappa}_1 \longrightarrow \mathrm{Image}\,\underline{\kappa}_2. \tag{5.3}$$

Since this diffeomorphism may be extended to a diffeomorphism g_{21} of $\mathscr{S}$, all elements $\underline{\kappa} \in \underline{\mathscr{Q}}$ are related. This implies that all $\underline{\kappa} \in \underline{\mathscr{Q}}$ share the same embodiment $\underline{e} = [\underline{\kappa}] \in \underline{\mathscr{E}}$, so that $\underline{\mathscr{E}} = \{\underline{e}\}$.

Moreover, as for any $\kappa \in \mathscr{Q}$, Image $\underline{\kappa}$ is diffeomorphic with $\mathscr{B}$ and diffeomorphic with the single $\mathscr{B}_{\underline{e}}$, we may naturally identify $\mathscr{B}_{\underline{e}}$ with $\mathscr{B}$ so that $\kappa_{\underline{ae}}$ is the identity. It follows that for every

κ, $\underline{\kappa_e} = \underline{\kappa}$, $\underline{\pi_{e\kappa}} = \underline{\kappa}^{-1}$: Image $\underline{\kappa} \to \mathscr{B}$, and Diagram (4.27) reduces to

$$\begin{tikzcd}
{} & {} & {} & \mathrm{Image}\,\kappa \subset T\mathscr{S} \arrow[dl, "\pi_{e\kappa}"'] \arrow[dd, "\xi_\kappa"] \\
T\mathscr{B} \arrow[urrr, "\kappa"] \arrow[rr, "\kappa_{ae}"] \arrow[ddr, "\tau_{\mathscr{B}}"'] & {} & W_e \arrow[ur, bend right, "\kappa_e"'] \arrow[ddl, "\pi_{W_e}"] & {} \\
{} & {} & {} & \mathrm{Image}\,\underline{\kappa} \subset \mathscr{S} \\
{} & \mathscr{B} = \underline{\mathscr{B}_e} \arrow[urr, "\underline{\kappa}"] & {} & {}
\end{tikzcd} \tag{5.4}$$

As mentioned above, the presence of dislocations, or incompatibility, is reflected by the fact that κ is different from $T\underline{\kappa}$.

Lemma 5.1. *Let $\kappa_1, \kappa_2 \in \mathscr{Q}$. Then, $\kappa_1 \sim \kappa_2$ if and only if*

$$(T\underline{\kappa}_1)^{-1} \circ \kappa_1 = (T\underline{\kappa}_2)^{-1} \circ \kappa_2, \tag{5.5}$$

where each side of the equation is a vector bundle morphism $T\mathscr{B} \to T\mathscr{B}$ over the identity, and left inverses of the tangent mappings are well-defined on the images of the configurations.

Proof. Assume that $\kappa_1 \sim \kappa_2$. Then, there is a diffeomorphism $g_{21} : \mathscr{S} \to \mathscr{S}$ such that $\underline{\kappa}_2 = g_{21} \circ \underline{\kappa}_1$ and $\kappa_2 = Tg_{21} \circ \kappa_1$. Hence,

$$\begin{aligned}
(T\underline{\kappa}_2)^{-1} \circ \kappa_2 &= (T(g_{21} \circ \underline{\kappa}_1))^{-1} \circ Tg_{21} \circ \kappa_1, \\
&= (Tg_{21} \circ T\underline{\kappa}_1)^{-1} \circ Tg_{21} \circ \kappa_1, \\
&= (T\underline{\kappa}_1)^{-1} \circ \kappa_1, \\
&= T\underline{\kappa}_1^{-1} \circ \kappa_1.
\end{aligned} \tag{5.6}$$

Conversely, assume that condition (5.5) holds. Then,

$$\begin{aligned}
\kappa_2 &= T\underline{\kappa}_2 \circ (T\underline{\kappa}_1)^{-1} \circ \kappa_1, \\
&= T\underline{\kappa}_2 \circ T\underline{\kappa}_1^{-1} \circ \kappa_1, \\
&= T(\underline{\kappa}_2 \circ \underline{\kappa}_1^{-1}) \circ \kappa_1.
\end{aligned} \tag{5.7}$$

As mentioned above, $\underline{\kappa}_1 \simeq \underline{\kappa}_2$ always, and so, there is an extending diffeomorphism $g_{21}: \mathscr{S} \to \mathscr{S}$ such that $\underline{\kappa}_2 \circ \underline{\kappa}_1^{-1}$ is the restriction of g_{21} to Image $\underline{\kappa}_1$ as in the following diagram

$$\begin{tikzcd}
 & & T\mathscr{B} \arrow[dll, "\kappa_1"'] \arrow[dl, "\kappa_2"] \arrow[dd, "\tau_{\mathscr{B}}"] \\
\text{Image}\,\kappa_1 \arrow[r, "T(\underline{\kappa}_2\circ\underline{\kappa}_1^{-1})"'] \arrow[dd, "\tau_{\mathscr{S}}"'] & \text{Image}\,\kappa_2 \arrow[dd, "\tau_{\mathscr{S}}"'] & \\
 & & \mathscr{B} \arrow[dll, "\underline{\kappa}_1"'] \arrow[dl, "\underline{\kappa}_2"] \\
\text{Image}\,\underline{\kappa}_1 \arrow[r, "\underline{\kappa}_2\circ\underline{\kappa}_1^{-1}"'] & \text{Image}\,\underline{\kappa}_2 &
\end{tikzcd} \tag{5.8}$$

It follows that $\kappa_2 = Tg_{21} \circ \kappa_1$. ∎

We conclude that for any embodiment $e = [\kappa]$, there is a unique oriented vector bundle isomorphism

$$F_{ae}: T\mathscr{B} \longrightarrow T\mathscr{B}, \tag{5.9}$$

over the identity of $\mathscr{B}$. For any $\kappa \in e$, F_{ae} satisfies

$$F_{ae} = (T\underline{\kappa})^{-1} \circ \kappa, \tag{5.10}$$

and this definition is independent of the choice of κ.

Consequently,

Proposition 5.2. *For a dislocated crystal, the embodiment space may be identified with the group of oriented vector isomorphisms $T\mathscr{B} \to T\mathscr{B}$, over the identity.*

Any such vector bundle isomorphism may be identified with a section of a principal fibre bundle over $\mathscr{B}$, the fibre at $X \in \mathscr{B}$ of which is $GL(T_X\mathscr{B})^+$. Evidently, under a chart, the fibre may be modelled by $GL(n)^+$, which also acts on the fibres (see [34, p. 313]). In fact, we obtain the material G-structure of [35, p. 261].

Remark 5.3. As mentioned in the Introduction, we view the plastic factor, κ_{ae}, of the decomposition as the vector bundle morphism that maps the perfect crystal structure to the dislocated one, an incompatible vector bundle morphism (as it not the tangent of the base mapping). The plastic factor is followed by a compatible (the tangent to the base map) vector bundle morphism $\kappa_e: \mathscr{B}_e \to \mathscr{S}$. Their composition gives the incompatible configuration of the protobody in space. For this remark, let us refer to this point of view as II, and write

$$\kappa^{II} = \kappa_e^{II} \circ \kappa_{ae}^{II}, \tag{5.11}$$

for a compatible κ_e^{II}.

This point of view differs from the point of view (e.g. [3]) where the body is first dissected into small neighbourhoods to release the residual stresses—an incompatible mapping—then packed into the new configuration in space by another incompatible mapping, so that the composition is a compatible vector bundle morphism of the body into space. Let us refer to this point of view as I and write

$$\kappa^{I} = \kappa_e^{I} \circ \kappa_{ae}^{I}, \tag{5.12}$$

where now κ^I is compatible.

The relation between the two points of view is quite clear. If we make the identification

$$\kappa^I_{ae} = (\kappa^{II}_{ae})^{-1} : \mathscr{B}_e \longrightarrow T\mathscr{B} \quad \text{and} \quad \kappa^I_e = \kappa^{II} : T\mathscr{B} \longrightarrow T\mathscr{S}, \tag{5.13}$$

we obtain

$$\kappa^I = \kappa^{II} \circ (\kappa^{II}_{ae})^{-1}, \tag{5.14}$$

as in the following diagram.

$$\begin{tikzcd}
 & \mathrm{Image}\,\kappa \subset T\mathscr{S} \\
T\mathscr{B} \arrow[ur, "\kappa^{II}=\kappa^{I}_{e}"] \arrow[r, "\kappa^{II}_{ae}"] & \mathscr{B}_e. \arrow[u, "\kappa^{I}=\kappa^{II}_{e}"'] \arrow[l, bend left, "\kappa^{I}_{ae}=(\kappa^{II}_{ae})^{-1}"]
\end{tikzcd} \tag{5.15}$$

While in point of view I, the basic object is the 'frustrated' body $\mathscr{B}_e$, for view II, which we adopt in this manuscript, the basic object is $T\mathscr{B}$, interpreted as the perfect crystal.

6. Dislocated quasi-crystals

The above construction admits a natural adaptation to the case of quasi-crystals, i.e. those (natural and synthetic) alloys showing a quasi-periodic distribution of Bragg's peaks under diffraction experiments. In fact, every n-dimensional quasi-periodic lattice can be considered as the projection of a periodic atomic array in a $2n$-dimensional space onto a n-dimensional incommensurate subspace. For example, consider a quasi-periodic lattice in the plane and develop the mass density function in a Fourier series; quasi-periodicity imposes in the Fourier series a four-dimensional wave vector: once again we go from n to $2n$ [36].

Quasi-crystals admit dislocations [37,38]. Their Burgers vector admits a component in the incommensurate subspace and another one in the orthogonal complement to that space in the higher-dimensional space from which we construct the quasi-periodic lattice [39,40].

To exploit in this case the structure in the previous section, we could consider $\mathscr{B}$ itself as a locally trivial fibre bundle with base manifold a fit region in three-dimensional real space and $\mathbb{R}^3$ as a typical fibre. The fit region includes the physical atoms constituting the body, while the fibre at each point includes information on the low-scale atomic flips that assure quasi-periodicity in the physical space. Then we consider $T\mathscr{B}$ and act as above, paying attention to the circumstance that equivalence relations should account for both basis and fibre of $\mathscr{B}$ at the same time; in essence they can be considered as those in the previous section when referred to the higher-dimensional space from which we obtain the quasi-periodic lattice.

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