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On the Dynamics of Continuous Distributions of Dislocations

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On the Dynamics of Continuous Distributions of Dislocations

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Abstract

For materials with a continuous distribution of dislocations, equations of motion are derived from a symplectic structure on an appropriate configuration space. The proposed dynamics generalizes from elasticity.

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1 Introduction

A mathematical framework for the dynamics of an elastic material is given by the space of all embeddings $E(M;\mathbb{R}^3)$ of a reference body M into the physical space $\mathbb{R}^3$. The constitutive law determining the equations of evolution can be given in terms of a virtual work functional on this phase space, cf. [8]. The invariance of the system under rigid global translations implies that the differential dj of the embedding $j \in E(M;\mathbb{R}^3)$ is the essential quantity for the constitutive behaviour of the material, cf. [3]. In classical terms this differential is precisely the deformation gradient of the actual configuration of the system. Mathematically the deformation gradient dj may be considered as an exact ($\mathbb{R}^3$-valued) differential one-form in $\Omega^1(M;\mathbb{R}^3)$.

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In the continuum theory of defects one describes dislocations by a torsion density on the reference body, cf. [9, 15, 19]. This torsion density may be identified with an exact ($\mathbb{R}^3$-valued) differential two-form $d\gamma \in \Omega^2(M; \mathbb{R}^3)$. The corresponding Burgers vector computes as the integral of $d\gamma$ over a bounded surface $S \subset M$, cf. [20].

To incorporate this describtion of dislocations into the framework of elasticity, the Helmholtz decomposition theorem is utilized which claims that any differential form may be uniquely decomposed into a gradient and a divergence-free part. A generalised configuration space for a material with dislocations $\mathcal{V}(M; \mathbb{R}^3)$ is defined as a submanifold of $\Omega^1(M; \mathbb{R}^3)$. Each generalised configuration $\gamma \in \mathcal{V}(M; \mathbb{R}^3)$ splits into an elastic or gradient part dj, where $j \in E(M; \mathbb{R}^3)$ is an embedding, and into a so-called plastic part β describing the dislocation density, cf. [20].

The main objective of this paper is to derive a dynamics for a material with a continuous distribution of dislocations. This is done by introducing a symplectic structure Ω and a kinetic engergy functional $\mathcal{E}$ on the tangent space $T\mathcal{V}(M; \mathbb{R}^3)$ of the configuration space $\mathcal{V}(M; \mathbb{R}^3)$. The constitutive behaviour of such a system is described by a virtual work functional F on $\mathcal{V}(M; \mathbb{R}^3)$. The resulting principle of virtual work determines weak equations of motion for the generalised configurations γ.

Using the Helmholtz decomposition theorem, these equations split into a part which determines the evolution of the elastic parts dj of a generalised configuration γ and into a part which determines the evolution of the plastic parts β. The equations for the elastic parts are just the well-known equations in classical elasticity. Thus, for purely elastic materials, this approach covers the classical theory.

2 Differential Forms

Since in this approach towards a dynamics of dislocations, differential forms provide a convenient framework, a brief introduction is given. Let M be the *body manifold* in the sense of elasticity. Assume that M is a smooth connected 3-dimensional compact oriented Riemannian manifold with boundary which is embedable into the physical space $\mathbb{R}^3$. A $\mathbb{R}^3$-valued differential form $\omega \in \Omega^k(M; \mathbb{R}^3)$ of degree k is a smooth assignment of a skew-symmetric k-linear map ω_p on T_pM to each point $p \in M$, where

$$\omega_p : \underbrace{T_pM \times \cdots T_pM}_{k-times} \longrightarrow \mathbb{R}^3 \quad \forall p \in M.$$

In classical terms, differential forms may be considered as skew-symmetric two-point tensors of type $(1, k)$ on the body manifold M which are well-known objects in continuum mechanics, cf. [12]. Of particular interest in our approach are the cases $k = 0, 1, 2$. For example, the deformation gradient and the first Piola-Kirchoff stress tensor are considered here as $\mathbb{R}^3$-valued one-forms on the body manifold M, i.e. as some $\omega \in \Omega^1(M;\mathbb{R}^3)$. Analogously, placements of M and force fields are elements in $\Omega^0(M;\mathbb{R}^3)$ which, by definition, is equal to $C^\infty(M;\mathbb{R}^3)$.

Each $\Omega^k(M;\mathbb{R}^3)$ may be equipped with a fibre metric by using the Riemannian metric g on M and the standard scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^3}$ on $\mathbb{R}^3$. For our purposes, it suffices to consider the cases $k=0,1$. Let $E_1,E_2,E_3 \in \Gamma(TM)$ be a triple of vector fields orthonormal with respect to the metric g. A fibre metric on $\Omega^1(M;\mathbb{R}^3)$ is then defined by

$$\langle\omega,\eta\rangle := \sum_i \langle\omega(E_i),\eta(E_i)\rangle_{\mathbb{R}^3}, \quad \omega,\eta \in \Omega^1(M;\mathbb{R}^3). \tag{1}$$

The product (1) does only depend on the metric g but not on the chosen frame on M, cf. [13]. Notice that (1) corresponds to the contraction of skew symmetric two-point tensors. If $e_1,e_2,e_3 \in \mathbb{R}^3$ denotes the standard basis in $\mathbb{R}^3$ and $\theta^1,\theta^2,\theta^3 \in \Omega^1(M)$ the dual frame corresponding to E_1,E_2,E_3, then, in coordinates, any one-forms ω and η may be written as $\omega = \sum_{L,l}\omega_l^L\theta^l e_L$ and $\eta = \sum_{L,l}\eta_l^L\theta^l e_L$. Thus (1) reads

$$\langle\omega,\eta\rangle = \sum_{L,l=1}^{3} \omega_l^L\eta_l^L.$$

With the help of the Riemannian volume element μ induced by g, the space $\Omega^1(M;\mathbb{R}^3)$ is now endowed with an L^2-product $\mathcal{G}$, given by

$$\mathcal{G}(\omega,\eta) := \int_M \langle\omega,\eta\rangle\mu, \quad \omega,\eta \in \Omega^1(M;\mathbb{R}^3). \tag{2}$$

For $k=0$ the corresponding L^2-product $\mathcal{G}$ is just the usual one. Let ∇ denote the Levi-Civita connection on M associated to g. Then ∇ induces a *covariant derivative* on $\Omega^1(M;\mathbb{R}^3)$, given by

$$(\nabla_Y\omega)(X) = D[\omega(X)](Y) - \omega(\nabla_Y X), \quad X,Y \in \Gamma(TM).$$

Here, the first term of the right hand side means the directional derivative of the $\mathbb{R}^3$-valued function $\omega(X)$ in direction of the vector field Y. For $k=0$ the second term of the right hand side of the above expression vanishes. The covariant derivative allows to write the *exterior derivative* $d:\Omega^1(M;\mathbb{R}^3) \longrightarrow \Omega^2(M;\mathbb{R}^3)$ as

$$d\omega(X,Y) = (\nabla_X\omega)(Y) - (\nabla_Y\omega)(X), \quad X,Y \in \Gamma(TM).$$

For $k=0$ the exterior derivative corresponds to the gradient. The *co-differential* $\delta : \Omega^1(M;\mathbb{R}^3) \longrightarrow \Omega^0(M;\mathbb{R}^3)$ may be defined by

$$\delta\omega := -\sum_{i=1}^{3}(\nabla_{E_i}\omega)(E_i).$$

Notice that the co-differential δ, unlike the exterior derivative, depends on the chosen Riemannian metric g. In classical tensor notation, δ corresponds to the divergence of a tensor field.

Let $\mathcal{N}$ denote the outward pointing unit normal field on the boundary ∂M of M. A differential one-form ω is called *parallel* to ∂M iff its normal component vanishes, that is $\omega(\mathcal{N}) = 0$. Define the space of all divergence-free and parallel one-forms by

$$\mathcal{D}(M; I\!R^3) := \left\{\omega \in \Omega^1(M; I\!R^3) \mid \delta\omega = 0 \text{ and } \omega(\mathcal{N}) = 0\right\}.$$

We are now able to state the *Helmholtz decomposition* for the special case of $I\!R^3$-valued one-forms. For a general proof see [17].

Theorem 2.1 HELMHOLTZ DECOMPOSITION
Let M be a compact, oriented Riemannian manifold with boundary. Then for any $\omega \in \Omega^1(M; I\!R^3)$ there exist $\theta \in \Omega^0(M; I\!R^3)$ and $\beta \in \mathcal{D}(M; I\!R^3)$ such that $\omega = d\theta + \beta$. Moreover, $d\theta$ and β are mutually L^2-orthogonal with respect to the inner product (2), that is the decomposition

$$\Omega^1(M; I\!R^3) = d\Omega^0(M; I\!R^3) \oplus \mathcal{D}(M; I\!R^3)$$

is direct and L^2-orthogonal.

3 The Kinematics of Dislocations

Let $j : M \longrightarrow I\!R^3$ be a smooth embedding of the body manifold M into the Euclidean space $I\!R^3$, and $E(M; I\!R^3)$ denote the space of all such embeddings[1]. In pure elasticity $E(M; I\!R^3)$ constitutes the configuration space of the system; in classical terms its elements j are called placement (or transplacement) fields. The displacement fields $u \in C^\infty(M; I\!R^3)$ compute as $u = (j - j_0)$, where j_0 is a reference configuration.

This section is aimed at generalising the classical configuration space $E(M; I\!R^3)$ in such a way that the description of the kinematics of dislocations is included. We introduce a configuration space for an elastic solid whose internal structure is characterised by a frame, i.e. a triple of linear independent vector fields on M

$$Y_1, Y_2, Y_3 \in \Gamma(TM). \tag{3}$$

Physically, these vector fields describe lattice vectors of a continuised crystal as worked out in [9]. We denote the standard basis of $I\!R^3$ by e_1, e_2, e_3. Since M is embedable

[1] $E(M; I\!R^3)$ is an open subset in the Fréchet space $C^\infty(M; I\!R^3)$, see [2] for details.

into $I\!R^3$, for any arbitrary frame (3), there exists a unique fibrewise one-to-one map $\gamma : TM \longrightarrow I\!R^3$ such that

$$\gamma_p(Y_i(p)) = e_i, \quad i = 1, 2, 3 \quad \forall p \in M. \tag{4}$$

Mathematically, γ is a $I\!R^3$-valued one-form $\gamma \in \Omega^1(M; I\!R^3)$ on M which is fibrewise one-to-one. The set of all these one-forms is defined by

$$\mathcal{I}(M; I\!R^3) := \left\{ \gamma \in \Omega^1(M; I\!R^3) \mid \gamma_p : T_pM \longrightarrow I\!R^3 \text{ is one-to-one, } p \in M \right\}.$$

Consider a fixed $\gamma \in \mathcal{I}(M; I\!R^3)$. Then $\gamma(X) \in C^\infty(M; I\!R^3)$ is a smooth function for each $X \in \Gamma(TM)$. Let $D(\gamma(X))(Y)$ denote the directional derivative of $\gamma(X)$ into the direction of some $Y \in \Gamma(TM)$. A connection $\nabla[\gamma]$ on TM associated with $\gamma \in \mathcal{I}(M; I\!R^3)$ is then defined by

$$\nabla[\gamma]_Y X = \gamma^{-1} D(\gamma(X))(Y), \quad X, Y \in \Gamma(TM). \tag{5}$$

In a coordinate system on M, the Christoffel symbols of (5) read

$$\Gamma^k_{lm} = \sum_{L=1}^{3} (\gamma^{-1})^k_L \partial_l \gamma^L_m.$$

It is easy to verify that the curvature of this connection vanishes, i.e. the connection (5) is flat. Conversely, it is shown in [20] that for any flat connection $\widetilde{\nabla}$ on TM, there is some $\gamma \in \mathcal{I}(M; I\!R^3)$ with $\widetilde{\nabla} = \nabla[\gamma]$. The torsion T^∇ of an arbitrary connection ∇ is defined by

$$T^\nabla(X, Y) = \nabla_Y X - \nabla_X Y - [X, Y] \quad \forall X, Y \in \Gamma(TM).$$

In particular, if $T[\gamma]$ denotes the torsion of $\nabla[\gamma]$, it follows from (5) and the definition of the exterior derivative d that

$$d\gamma(X, Y) = \gamma(T[\gamma](X, Y)), \quad X, Y \in \Gamma(TM).$$

In classical terms, the torsion of a connection describes the *dislocation density* or the *material inhomogeneity* of a material. Since γ is fibrewise one-to-one, the discussion shows that $T[\gamma] = \gamma^{-1} d\gamma$. Therefore, the dislocation density $T[\gamma]$ might as well be measured by the exterior derivative of the one-form $\gamma \in \mathcal{I}(M; I\!R^3)$. Hence, the two-form $d\gamma$ will be referred to as a dislocation density of the material. In particular,

$$d\gamma = 0 \quad \Longleftrightarrow \quad T[\gamma] = 0,$$

implying that the material is defect-free if and only if γ is closed, i.e. $d\gamma = 0$. The Burgers vector b of an arbitrary surface $S \subset M$ associated with the dislocation density $d\gamma$ computes as the integral

$$b = \int_S d\gamma.$$

The crucial observation is that according to the *Helmholtz decomposition*, Theorem 2.1, each $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ uniquely splits into

$$\gamma = dv + \beta, \quad \text{where} \quad dv \in d\Omega^0(M; \mathbb{R}^3), \quad \beta \in \mathcal{D}(M; \mathbb{R}^3). \tag{6}$$

Since $d^2 = 0$, only the divergence-free part $\beta \in \mathcal{D}(M; \mathbb{R}^3)$ of γ contributes to the dislocation density. In particular $d\gamma = d\beta$, i.e. the dislocation density is uniquely determined by the so-called non-exact component β.

As far as classical elasticity is concerned, the essential quantity for the constitutive behaviour of a material is the deformation gradient $dj \in \Omega^1(M; \mathbb{R}^3)$ of an actual embedding $j \in E(M; \mathbb{R}^3)$. It is shown in [3] that the set of all such gradients

$$dE(M; \mathbb{R}^3) = \left\{ dj \mid j \in E(M; \mathbb{R}^3) \right\}$$

is an open subset of the Fréchet space of all one-forms $\Omega^1(M; \mathbb{R}^3)$. Since differentials of embeddings are fibrewise one-to-one, we have $dE(M; \mathbb{R}^3) \subset \mathcal{I}(M; \mathbb{R}^3)$. Each deformation gradient $dj \in dE(M; \mathbb{R}^3)$ defines a frame $X_1, X_2, X_3 \in \Gamma(TM)$ by solving

$$dj(X_l) = e_l, \qquad l = 1, 2, 3. \tag{7}$$

Since $d^2 = 0$, it follows from (4) that this triple of vector fields characterises a defect-free material. Therefore, a placement $j \in E(M; \mathbb{R}^3)$ will be called *integrable configuration* of the body manifold M; an arbitrary $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ will be referred to as a *generalised configuration* of M.

According to [18] the evolution of defects is held responsible for the discrepancy between the macroscopic deformation and the behaviour of the lattice. Therefore, we think of the component $\beta \in \mathcal{D}(M; \mathbb{R}^3)$ as a quantity by which the frame X_1, X_2, X_3 is *incompatibly* deformed. The vector fields

$$(dj + \beta)(X_1), (dj + \beta)(X_2), (dj + \beta)(X_3)$$

constitute a frame on $j(M) \subset \mathbb{R}^3$ if and only if $dj + \beta$ is injective. For $\beta \neq 0$, this frame represents a dislocated lattice on the embedded body.

The general idea is that only the integrable part, i.e. the gradient part of a generalised configuration $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ becomes visible as a placement of the body manifold in Euclidean space. Thus, we consider generalised configurations $\gamma = dj + \beta \in \mathcal{I}(M; \mathbb{R}^3)$ whose integrable part dj stems from a placement $j \in E(M; \mathbb{R}^3)$ and whose non-integrable part β lies in $\mathcal{D}(M; \mathbb{R}^3)$. The set of all such configurations is denoted by

$$\mathcal{V}(M; \mathbb{R}^3) = \left\{ dj + \beta \in \mathcal{I}(M; \mathbb{R}^3) \mid j \in E(M; \mathbb{R}^3), \beta \in \mathcal{D}(M; \mathbb{R}^3) \right\}.$$

Observe that by construction $\mathcal{V}(M; \mathbb{R}^3) \subset \mathcal{I}(M; \mathbb{R}^3)$, where the exact parts of generalised configurations $\gamma \in \mathcal{V}(M; \mathbb{R}^3)$ are restricted to embeddings $j \in E(M; \mathbb{R}^3)$. Since $\mathcal{V}(M; \mathbb{R}^3)$ is an open Fréchet submanifold of $\Omega^1(M; \mathbb{R}^3)$, we take $\mathcal{V}(M; \mathbb{R}^3)$ as a configuration space for an elastic material which possibly may be dislocated, cf. [20].

4 The Geometry of $\mathcal{V}(M;\mathbb{R}^3)$

For a mathematical formulation of a dynamic theory of dislocated materials, a metric on the configuration space $\mathcal{V}(M;\mathbb{R}^3)$ is needed. Following [6], we first introduce an appropriate metric on $dE(M;\mathbb{R}^3)$. Let $\rho : M \longrightarrow \mathbb{R}$ be a strictly positive real-valued function which physically may be thought of as the mass distribution of the material. Since $E(M;\mathbb{R}^3)$ is open in $C^\infty(M;\mathbb{R}^3)$, the tangent manifold of $E(M;\mathbb{R}^3)$ is trivial

$$TE(M;\mathbb{R}^3) = E(M;\mathbb{R}^3) \times C^\infty(M;\mathbb{R}^3).$$

Identifying each tangent vector with its principal part, a metric on $E(M;\mathbb{R}^3)$ is defined by setting

$$\mathcal{G}_\rho(u_1,u_2) := \int_M \rho\langle u_1,u_2\rangle_{\mathbb{R}^3}\mu, \quad u_1,u_2 \in C^\infty(M;\mathbb{R}^3). \tag{8}$$

Using (8), each $j \in E(M;\mathbb{R}^3)$ and each $u \in C^\infty(M;\mathbb{R}^3)$ may be decomposed into

$$j = j^0 + C_j, \quad \text{where} \quad C_j \in \mathbb{R}^3, \quad \mathcal{G}_\rho(j^0,c) = 0 \quad \forall c \in \mathbb{R}^3$$

and

$$u = u^0 + C_u, \quad \text{where} \quad C_u \in \mathbb{R}^3, \quad \mathcal{G}_\rho(u^0,c) = 0 \quad \forall c \in \mathbb{R}^3$$

respectively. The sets

$$E_0(M;\mathbb{R}^3) := \left\{ j \in E(M;\mathbb{R}^3) \mid \int_M \rho j \,\mu = 0 \right\}$$

and

$$C_0^\infty(M;\mathbb{R}^3) := \left\{ u \in C^\infty(M;\mathbb{R}^3) \mid \int_M \rho u \,\mu = 0 \right\}$$

are Fréchet manifolds which are naturally isomorphic to $dE(M;\mathbb{R}^3)$ and $d\Omega^0(M;\mathbb{R}^3)$ respectively, cf. [3, 4]. Since $dE(M;\mathbb{R}^3) \subset d\Omega^0(M;\mathbb{R}^3)$ is open,

$$T(dE(M;\mathbb{R}^3)) = dE(M;\mathbb{R}^3) \times d\Omega^0(M;\mathbb{R}^3).$$

Configurations in $j \in E_0(M;\mathbb{R}^3)$ are such that the center of mass is kept fixed, $C_j = 0$. A metric on $dE(M;\mathbb{R}^3)$ naturally induced by this construction is given by

$$\mathcal{G}_E(du_1,du_2) := \int_M \rho\langle u_1^0,u_2^0\rangle_{\mathbb{R}^3}\mu, \quad du_1,du_2 \in d\Omega^0(M;\mathbb{R}^3), \tag{9}$$

where we identify tangent vectors with their principal parts.

As the configuration space $\mathcal{V}(M;\mathbb{R}^3)$ is an open subset of $\Omega^1(M;\mathbb{R}^3)$, the tangent manifold $T\mathcal{V}(M;\mathbb{R}^3)$ of $\mathcal{V}(M;\mathbb{R}^3)$ is trivial

$$T\mathcal{V}(M;\mathbb{R}^3) = \mathcal{V}(M;\mathbb{R}^3) \times \Omega^1(M;\mathbb{R}^3).$$

Applying Theorem 2.1, tangent vectors $\eta \in T\mathcal{V}(M;\mathbb{R}^3)$ allows to equip the configuration space $\mathcal{V}(M;\mathbb{R}^3)$ with a metric as follows.

Definition 4.1 Let $\gamma \in \mathcal{V}(M; I\!R^3)$ be an arbitrary generalised configuration. For each pair $\eta_i \in T_\gamma \mathcal{V}(M; I\!R^3)$, $i = 1, 2$, let

$$\eta_i = du_i + v_i \quad \text{with} \quad du_i \in d\Omega^0(M; I\!R^3), \; v_i \in \mathcal{D}(M; I\!R^3)$$

be the respective Helmholtz decompositions. A metric $\mathcal{G}_\mathcal{V}$ on the configuration space $\mathcal{V}(M; I\!R^3)$ is defined by setting

$$\mathcal{G}_\mathcal{V}[\gamma](\eta_1, \eta_2) := \mathcal{G}_\mathcal{V}^{(e)}[\gamma](du_1, du_2) + \mathcal{G}_\mathcal{V}^{(p)}[\gamma](v_1, v_2).$$

The *elastic* part of $\mathcal{G}^{(e)}$ is given by

$$\mathcal{G}_\mathcal{V}^{(e)}[\gamma](du_1, du_2) := \mathcal{G}_E(du_1, du_2), \quad du_1, du_2 \in d\Omega^0(M; I\!R^3),$$

where $\mathcal{G}_E$ is defined in (9). The *plastic* part of $\mathcal{G}_\mathcal{V}$ is given by

$$\mathcal{G}_\mathcal{V}^{(p)}[\gamma](v_1, v_2) := \int_M \sigma \langle v_1, v_2 \rangle \mu, \quad v_1, v_2 \in \mathcal{D}(M; I\!R^3),$$

where $\sigma \in C^\infty(M)$ is a strictly positive real-valued function.

Notice that physically, the function σ appearing in the above metric may be thought of as the density of inertia of the dislocations. For sake of simplicity we assume that the density σ is independent of the actual configuration. This means that all dislocations respond to a force action by the same specific inertia.

Let $T\tau_\mathcal{V} : T^2\mathcal{V}(M; I\!R^3) \longrightarrow T\mathcal{V}(M; I\!R^3)$ denote the tangent map of the canonical projection $\tau_\mathcal{V}$ and $V(T\mathcal{V}(M; I\!R^3)) := \ker T\tau_\mathcal{V}$ the vertical bundle. Moreover, let $V\mathcal{X} \in V(T\mathcal{V}(M; I\!R^3))$ denote the vertical component of any vector $\mathcal{X} \in T^2\mathcal{V}(M; I\!R^3)$. The metric $\mathcal{G}_\mathcal{V}$ given in Definition 4.1 defines a natural weakly nondegenerate symplectic two-form Ω on $T\mathcal{V}(M; I\!R^3)$ by

$$\Omega[\xi](\mathcal{X}, \mathcal{Y}) := \mathcal{G}_\mathcal{V}[\gamma](V\mathcal{Y}, T\tau_\mathcal{V}\mathcal{X}) - \mathcal{G}_\mathcal{V}[\gamma](V\mathcal{X}, T\tau_\mathcal{V}\mathcal{Y}) \tag{10}$$

for all $\mathcal{X}, \mathcal{Y} \in T_\xi T\mathcal{V}(M; I\!R^3)$, $\xi \in T_\gamma \mathcal{V}(M; I\!R^3)$, $\gamma \in \mathcal{V}(M; I\!R^3)$. Thus, $T\mathcal{V}(M; I\!R^3)$ endowed with Ω becomes a symplectic manifold. Since $T\mathcal{V}(M; I\!R^3)$ is trivial, in coordinates one has

$$\mathcal{X} = (\gamma, \xi, \xi_1, \xi_2) \quad \text{and} \quad \mathcal{Y} = (\gamma, \xi, \eta_1, \eta_2)$$

which in turn yields

$$\Omega[\gamma, \xi]((\xi_1, \xi_2), (\eta_1, \eta_2)) = \mathcal{G}_\mathcal{V}[\gamma](\eta_2, \xi_1) - \mathcal{G}_\mathcal{V}[\gamma](\xi_2, \eta_1).$$

The metric $\mathcal{G}_\mathcal{V}$ induces the kinetic energy functional $\mathcal{E} : T\mathcal{V}(M;\mathbb{R}^3) \longrightarrow \mathbb{R}$ of the dislocated material by setting

$$\mathcal{E}(\xi) := \frac{1}{2}\mathcal{G}_\mathcal{V}[\gamma](\xi,\xi), \quad \xi \in T_\gamma\mathcal{V}(M;\mathbb{R}^3), \quad \gamma \in \mathcal{V}(M;\mathbb{R}^3). \tag{11}$$

If $\xi = du + v$ denotes the Helmholtz decomposition, then, according to Definition 4.1, the kinetic energy $\mathcal{E}$ of a dislocated material splits into an *elastic part*

$$\mathcal{E}^{(e)}(\xi) := \frac{1}{2}\mathcal{G}_\mathcal{V}^{(e)}[\gamma](du,du),$$

corresponding to the kinetic energy associated with the material mass density, and into a *plastic part*

$$\mathcal{E}^{(p)}(\xi) := \frac{1}{2}\mathcal{G}_\mathcal{V}^{(p)}[\gamma](v,v),$$

corresponding to the kinetic energy of the dislocation density. By construction, the metric $\mathcal{G}_\mathcal{V}$ is constant in γ, that is

$$D\mathcal{G}_\mathcal{V}[\gamma](\eta) = 0 \quad \forall \eta \in T_\gamma\mathcal{V}(M;\mathbb{R}^3), \ \gamma \in \mathcal{V}(M;\mathbb{R}^3).$$

Therefore, the corresponding Euler's equations yield

$$\mathcal{G}_\mathcal{V}[\gamma(t)](\ddot{\gamma}(t),\eta) = 0, \quad \forall \eta \in T\mathcal{V}(M;\mathbb{R}^3)$$

as weak equations of motion. The geodesics of $\mathcal{G}_\mathcal{V}$ are analogously to elasticity straight line segments, cf. [4, 6]. An inertial motion follows by definition the geodesics of $\mathcal{G}_\mathcal{V}$. A motion under non-vanishing forces will deviate from these geodesics.

5 The Principle of Virtual Work

In our setting, a work functional on the space of generalised configurations $\mathcal{V}(M;\mathbb{R}^3)$ is understood to be a continuous linear functional

$$F : T\mathcal{V}(M;\mathbb{R}^3) \equiv \mathcal{V}(M;\mathbb{R}^3) \times \Omega^1(M;\mathbb{R}^3) \longrightarrow \mathbb{R},$$

on the tangent bundle $T\mathcal{V}(M;\mathbb{R}^3)$. We assume that for each configuration $\gamma \in \mathcal{V}(M;\mathbb{R}^3)$ the functional F admits an integral representation with respect to the metric $\mathcal{G}$ given in (2), such that

$$F[\gamma](\eta) = \int_M \langle \alpha[\gamma], \eta \rangle \mu \quad \forall \eta \in T_\gamma\mathcal{V}(M;\mathbb{R}^3). \tag{12}$$

The *constitutive law* of the continuum M is encoded in the functional dependence of the integral kernel $\alpha[\gamma] \in \Omega^1(M;\mathbb{R}^3)$ on the configuration γ. This dependence will, in general, be non-linear and possibly also non-local. More precisely, the integral kernel α may be thought of as a smooth section into the tangent bundle $T\mathcal{V}(M;\mathbb{R}^3)$, where each $\alpha[\gamma]$ is identified with its principal part. The one-form α will be called *stress form*; in classical elasticity, α corresponds to the *first Piola-Kirchhoff* stress tensor, cf. [5, 16].

For each $\gamma \in \mathcal{V}(M;\mathbb{R}^3)$, the Helmholtz decomposition of $\alpha[\gamma]$ reads

$$\alpha[\gamma] = dh[\gamma] + \tau[\gamma], \tag{13}$$

where $dh[\gamma] \in d\Omega^0(M;\mathbb{R}^3)$ is a gradient and $\tau[\gamma] \in \mathcal{D}(M;\mathbb{R}^3)$ is divergence-free. The decompositions are understood with respect to a fixed reference metric g. Writing $\eta = du + v$, the orthogonality of the Helmholtz decomposition implies

$$\mathcal{G}(\alpha[\gamma],\eta) = \mathcal{G}(dh[\gamma], du) + \mathcal{G}(\tau[\gamma], v).$$

Therefore, for each generalised configuration $\gamma \in \mathcal{V}(M;\mathbb{R}^3)$, the work functional F splits into an *elastic part* $F^{(e)}$ and a *plastic part* $F^{(p)}$, i.e.

$$F[\gamma](\eta) = F^{(e)}[\gamma](du) + F^{(p)}[\gamma](v) \quad \forall \eta = du + v \in T_\gamma\mathcal{V}(M;\mathbb{R}^3). \tag{14}$$

The elastic part is given by

$$F^{(e)}[\gamma](du) := \int_M \langle dh[\gamma], du\rangle \mu \qquad \forall du \in d\Omega^0(M;\mathbb{R}^3), \tag{15}$$

and the plastic part by

$$F^{(p)}[\gamma](v) := \int_M \langle \tau[\gamma], v\rangle \mu \qquad \forall v \in \mathcal{D}(M;\mathbb{R}^3). \tag{16}$$

Since the Helmholtz decomposition is orthogonal,

$$F = F^{(e)} \quad \Longleftrightarrow \quad \alpha[\gamma] = dh[\gamma] \quad \forall \gamma \in \mathcal{V}(M;\mathbb{R}^3).$$

It was first observed in [3] that in pure elasticity, only the exact part $dh[\gamma]$ of the stress form $\alpha[\gamma]$ contributes to the work functional. In fact, $F^{(e)}$ is the well-known work functional of elasticity, cf. [1, 7, 14]. The work functional (12) thus becomes a natural generalisation of the notion of work in classical elasticity.

Notice that both components $dh[\gamma]$ and $\tau[\gamma]$ of the stress form $\alpha[\gamma] = dh[\gamma] + \tau[\gamma]$ will, in general, depend on the integrable part dj as well as the plactic part $\beta \in \mathcal{D}(M;\mathbb{R}^3)$ of $\gamma = dj + \beta$. From the elastic point of view, τ marks a gauge freedom, cf. [5]. Hence, the choice of τ describes the plastic part in view.

Next, we implement the work functional (12) in the d'Alembert principle of virtual work. According to [13], an exterior force acting on a general mechanical system is given by a horizontal one-form on the tangent manifold of the corresponding configuration space.

Recall that, using the tangent map $T\tau_{\mathcal{V}} : T^2\mathcal{V}(M; I\!R^3) \longrightarrow T\mathcal{V}(M; I\!R^3)$ of the canonical projection $\tau_{\mathcal{V}}$, a vector field $\mathcal{Y}$ on $T\mathcal{V}(M; I\!R^3)$ is by definition *vertical* iff $T\tau_{\mathcal{V}}(\mathcal{Y}) = 0$. A one-form $\mathcal{F}$ on $T\mathcal{V}(M; I\!R^3)$ is *horizontal* iff $\mathcal{F}(\mathcal{Y}) = 0$ for all vertical vector fields $\mathcal{Y}$. Thus, an exterior force in the above sense acting on dislocated material is given by a horizontal one-form $\mathcal{F}$ on $T\mathcal{V}(M; I\!R^3)$.

If $\mathcal{Y}$ is a vertical vector field and Ω is the symplectic two-form defined in (10), then

$$\Omega(\mathcal{Y}, \mathcal{Z}) = -\mathcal{G}_{\mathcal{V}}[\gamma](\mathcal{Y}, T\tau_{\mathcal{V}}\mathcal{Z}) \quad \forall \mathcal{Z} \in \Gamma(T^2\mathcal{V}(M; I\!R^3)).$$

Therefore, the induced one-form $\imath_{\mathcal{Y}}\Omega$ given by

$$\imath_{\mathcal{Y}}\Omega(\mathcal{Z}) := \Omega(\mathcal{Y}, \mathcal{Z}) \quad \forall \mathcal{Z} \in \Gamma(T^2\mathcal{V}(M; I\!R^3))$$

is horizontal[2]. On the other hand, using the tangent map $T\tau_{\mathcal{V}}$ of the canonical projection $\tau_{\mathcal{V}}$, the work functional F defined in (12) induces an exterior work one-form $\mathcal{F}$ in the above sense by setting

$$\mathcal{F} := (T\tau_{\mathcal{V}})^{\star} F. \tag{17}$$

Due to the pull-back construction, $\mathcal{F}$ is horizontal. Given the kinetic energy functional $\mathcal{E}$ and an exterior work one-form (17), the d'Alembert principle of virtual work now states that the Euler vector field $\mathcal{X}$ is determined by the equation

$$d\mathcal{E}(\mathcal{Z}) - \imath_{\mathcal{X}}\Omega(\mathcal{Z}) = (T\tau_{\mathcal{V}})^{\star} F(\mathcal{Z}) \quad \forall \mathcal{Z} \in \Gamma(T^2\mathcal{V}(M; I\!R^3)). \tag{18}$$

6 The Equations of Motion

In order to formulate a dynamics on our configuration space $\mathcal{V}(M; I\!R^3)$, consider a motion given by a smooth curve

$$\gamma : I\!R \longrightarrow \mathcal{V}(M; I\!R^3), \quad t \longmapsto \gamma(t).$$

Using the exterior work functional (17), the curve $\gamma(t)$ describes a motion subject to the d'Alembert principle of virtual work (18), if it satifies the weak equations of motion

$$\mathcal{G}_{\mathcal{V}}[\gamma(t)](\ddot{\gamma}(t), \eta) = F[\gamma(t)](\eta) \quad \forall \eta \in \Omega^1(M; I\!R^3). \tag{19}$$

According to Helmholtz, each $\gamma(t)$, $t \in I\!R$ decomposes into $\gamma(t) = dj(t) + \beta(t)$. The orthogonality of the splittings of the work functional $F = F^{(e)} + F^{(p)}$ and the metric

[2] In the case where Ω is regular, the converse also holds true: for any horizontal one-form $\mathcal{F}$, there is a vertical vector field $\mathcal{Y}_{\mathcal{F}}$ such that $\mathcal{F} = \imath_{\mathcal{Y}_{\mathcal{F}}}\Omega$.

$\mathcal{G}_\mathcal{V} = \mathcal{G}^{(e)}_\mathcal{V} + \mathcal{G}^{(p)}_\mathcal{V}$ given in Definition 4.1, respectively, implies that (19) is equivalent to the system of equations

$$\mathcal{G}^{(e)}_\mathcal{V}[\gamma(t)](d\ddot{j}(t), du) = F^{(e)}[\gamma(t)](du) \quad \forall du \in d\Omega^0(M; I\!R^3) \tag{20}$$

and

$$\mathcal{G}^{(p)}_\mathcal{V}[\gamma(t)](\ddot{\beta}(t), v) = F^{(p)}[\gamma(t)](v) \quad \forall v \in \mathcal{D}(M; I\!R^3). \tag{21}$$

Thus, the dynamical equations derived from the principle of virtual work split into an *elastic part* (20) and into a *plastic part* (21). In absence of all external volume and surface forces, the equations of motion[3] induced by (20) and (21) are given in the following theorem.

Theorem 6.1 Let $\alpha[\gamma] = dh[\gamma] + \tau[\gamma]$ be the Helmholtz decomposition of a stress form for a dislocated material. Then the equations of motion are given by

$$\begin{cases} \rho\ddot{j}(t) &= \Delta h[\gamma(t)] \\ \sigma\ddot{\beta}(t) &= \tau[\gamma(t)] \end{cases},$$

where $\gamma(t) = dj(t) + \beta(t)$ is the Helmholtz decomposition of $\gamma(t)$ and $\Delta := \delta \circ d$ is the Laplace operator on functions in $C^\infty(M; I\!R^3)$.

The first equation in Theorem 6.1 is nothing but the well-known equation of motion in elasticity: since $\delta\tau[\gamma] = 0$, the divergence of the stress form $\alpha[\gamma]$ corresponding to the first Piola-Kirchhoff stress tensor can be represented as the Laplace operator on functions, i.e. $\delta\alpha[\gamma] = \Delta h[\gamma]$. The second one is an evolution equation for the non-integrable parts of the deformation $\gamma(t)$. The equations of motion are coupled via the Helmholtz decomposition. The motion of dislocations may, in general, be accompanied by dissipative effects, cf. [11].

In a static setting, $\gamma \in \mathcal{V}(M; I\!R^3)$ is an equilibrium configuration if and only if

$$F[\gamma](\eta) = 0 \quad \forall \eta \in T_\gamma\mathcal{V}(M; I\!R^3)$$

which according to (14) is equivalent to

$$F^{(e)}[\gamma](du) = 0 \quad \forall du \in d\Omega^0(M; I\!R^3) \quad \text{and} \quad F^{(p)}[\gamma](v) = 0 \quad \forall v \in \mathcal{D}(M; I\!R^3).$$

[3]The equivalence of the weak equations and the strong equations follow from the fact, that the space of smooth differential forms is dense in an appropriate L^2-completion, cf. [17].

The *second Piola-Kirchhoff* stress tensor $\boldsymbol{S}[\gamma]$ associated with the stress form $\alpha[\gamma] \in \Omega^1(M; I\!R^3)$, $\gamma \in \mathcal{V}(M; I\!R^3)$ is given by

$$\boldsymbol{S}[\gamma](X,Y) := \langle \alpha[\gamma](X), \gamma(Y) \rangle_{I\!R^3}, \quad X, Y \in \Gamma(TM).$$

In pure elasticity, there is a gauge freedom in choosing the stress form. Since only the integrable part $dh[\gamma]$ of a stress form $\alpha[\gamma]$ contributes to the work functional of elasticity $F^{(e)}$, any stress form $\tilde{\alpha}[\gamma] = \alpha[\gamma] + \xi[\gamma]$ with arbitrary $\xi[\gamma] \in \mathcal{D}(M; I\!R^3)$ will give the same work functional $F^{(e)}$ and hence determine the same dynamics of the system, cf. [3]. In particular, one may chose $\xi[\gamma]$ such that the stress tensor $\tilde{\boldsymbol{S}}$ corresponding to $\tilde{\alpha}[\gamma]$ is symmetric, cf. [16].

In the dislocated case, this gauge freedom ist lost. Since the divergence-free part τ of the stress form α appears explicitly in the principle of virtual work (19), the stress tensor may not chosen to be symmetric. The concept of decomposing configurations $\gamma \in \mathcal{V}(M; I\!R^3)$ and stress forms $\alpha[\gamma] \in \Omega^1(M; I\!R^3)$, $\gamma \in \mathcal{V}(M; I\!R^3)$ is completely analogous to the concept of strain spaces and stress spaces in [10]. The integrable part of the deformation is the dual quantity to the integrable part of the stress, the non-integrable part of the deformation is the dual quantity to the non-integrable part of the stress.

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