Kinematics of defected material: a geometrical point of view

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Abstract :

We consider kinematics of a defected medium in terms of Riemann-Cartan geometry supposing nonholonomic transformation. Torsion tensor is identified with the dislocation density. For incompatible transformation the connection and metric tensor is modified in order to describe the new defected state of the current medium. At each point of the body \mathfrak{B} , a local frame is attached. A priori, transformations of the frames and material points behave independently. In our approach, the difference between them illustrates the creation of defects in the current configuration. In practice, there exists two independent mechanisms, the first mechanism is the ordinary dragging of vectors by means of the deformation gradient of the macro structure or the transformation of the point, Φ , represented by the tensor with entries $\mathbf{F} = D\Phi$, the second mechanism is the one associated with the transformation Ψ of the micro structure characterized by the frame.

Each configuration is defined by its torsion and curvature. The relation between reference and current curvature is expressed thanks the action of Ψ . From point of view, there are two types of strain: the first one measures the change of lengths and angles around our material point. The last one is associated to the modification of the local frames. Accordingly, an energy function may be obtained in the form $\Xi = \Xi_{\Phi} + \Xi_{\Psi}$ where Ξ_{Φ}, Ξ_{Ψ} are the macroscopic energy and the nonholonomic energy respectively. The relation with $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$ will be presented.

Key words: defected medium, Riemann-Cartan geometry, non-holonomic transformation.

1 Introduction

In classical continuum mechanics, one idealizes the body as a collection of material points, with each point assumed to be mathematical point. Here, a local frame is attached at each element too, it illustrates the lattice structure at this material point. A priori transformations of the frames and material points behave independently. Hence, undergoing small transformations, the material points may remain at the same position as before but the frames can change. In this study, the transformation of points is characterized by a C^1 regular map Φ . The transformation of vector fields is associated with Ψ . We suppose the incompatibility of motion of point and frame ($ie \ \Psi \neq D\Phi$) implies colorbluepotential distribution of defects in the current medium.

In the reference configuration the material body is considered as a manifold \mathcal{B} described by a metric Gand a connection ∇ compatible with the metric. Let g be the spatial metric of the spatial manifold \mathcal{S} , where the body \mathfrak{B} moves. After transformations, we define, in the first section, a connection $\overline{\nabla}$ and a new material metric \overline{g} on the deformed current state $\Phi(\mathfrak{B})$ such that $\overline{\nabla}$ is compatible with \overline{g} . The relation between reference and current curvature is expressed too thanks the action of Ψ , practically $\overline{R} = \Psi R$. In the next section, two distinct strains are introduced. The first one measures the change of lengths and angles between neighboring material points: $\mathbf{E} = \frac{1}{2}(\Phi^*g - G)$. The second one is associated to the modification of the local frames $\mathcal{E} = (\Psi - \mathbf{F})^*g$, with $\mathbf{F} = D\Phi$. This tensor vanishes if and only if we have performed a holonomic transformation. Accordingly, a total internal energy function may be obtained in the form $\Xi = \Xi_{\Phi} + \Xi_{\Psi}$ where Ξ_{Φ} , Ξ_{Ψ} are the macroscopic energy and the nonholonomic energy respectively. The relation with $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$ will be presented.

2 Mathematical Model

We denote $\{X^A\}$, $\{E_A\}$, $\{dX^A\}$ and $T\mathfrak{B}$ (resp $\{x^a\}$, $\{e_a\}$, $\{dx^a\}$ and $T\mathcal{S}$) the coordinate systems, basis tangent, its dual and tangent bundle defined on \mathfrak{B} (resp \mathcal{S}). Material transformation is defined by mapping $\Phi : \mathfrak{B} \to \mathcal{S}$ that is C^1 -regular (one-to-one and has inverse C^1) and a bundle mapping $\Upsilon : T\mathfrak{B} \to T\mathcal{S}, (X, W) \mapsto (\Phi(X), \Psi(X)W)$ where $X \in \mathfrak{B}, W \in T_X\mathfrak{B}, \Psi \in C^1$ and det $\Psi(X) > 0$.

Definition 2.1. Let $x = \Phi(X)$, and $u, v \in T_xS$, an induced material geometry $(\overline{g}, \overline{\nabla})$ on $\Phi(\mathfrak{B}) \subset S$, *is defined as*

$$\overline{g}(x)(u,v) = G(X)(\Psi^{-1}(x)u, \Psi^{-1}(x)v),
\overline{\nabla}_{v}u = \Psi(X)(\nabla_{\Phi^{*}(x)v}\Psi^{-1}(x)u).$$
(1)

Proof. We need to verify that $\overline{\nabla}$ satisfies the following relations:

where f is a smooth function and v, u, w are vector fields on $\Phi(\mathfrak{B})$. Indeed,

Lemma 2.2. The connection $\overline{\nabla}$ is compatible with the metric \overline{g} .

Proof. For f a smooth function on $\Phi(\mathfrak{B})$, we have

$$\nabla_{\Phi^*v}(f \circ \Phi) = \Phi^*v[f \circ \Phi] = \frac{\partial X^A}{\partial x^a} v^a \frac{\partial f \circ \Phi}{\partial X^A} = \frac{\partial X^A}{\partial x^a} v^a \frac{\partial f}{\partial x^b} \frac{\partial x^b}{\partial X^A} = v^a \frac{\partial f}{\partial x^a} = v[f] = \overline{\nabla}_v f. \quad (3)$$

Hence,

$$\overline{\nabla}_v \overline{g}(x)(w,u) = \nabla_{\Phi^*(x)v} G(X)(\Psi^{-1}(x)w, \Psi^{-1}(x)u).$$
(4)

Setting $V = \Phi^* v$, $U = \Psi^{-1} u$ and $W = \Psi^{-1} w$ with $\Phi^* = \mathbf{F}^{-1}$, we have,

$$\overline{g}(w, \overline{\nabla}_v u) + \overline{g}(\overline{\nabla}_v w, u) = G(W, \nabla_V U) + G(\nabla_V W, U) = \nabla_V G(W, U) = \overline{\nabla}_v \overline{g}(w, u)$$

An affine connection ∇ is said to be compatible with a metric G if $G(W, \nabla_V U) + G(\nabla_V W, U) = \nabla_V G(W, U)$ for all $U, V, W \in T\mathfrak{B}$ [3]. Therefore, we conclude that the connection $\overline{\nabla}$ is compatible with the metric \overline{g} , ie, $\overline{\nabla g} = 0$.

In terms of components, the mapping $\Psi(X) : T_X \mathfrak{B} \to T_x \mathcal{S}$ is $\Psi(X) = \Psi_A^a(X)e_a \otimes dX^A$, and its inverse $\Psi^{-1}(x) : T_x \mathcal{S} \to T_X \mathfrak{B}$, $\Psi^{-1}(x) = H_b^B(x)E_B \otimes dx^b$ such that $H_b^B(x)\Psi_B^a(X) = \delta_b^a$. For all $u, v \in T_x \mathcal{S}$. Accordingly:

$$\overline{g}(x)(u,v) = H^A_a H^B_b u^a v^b G(X)_{AB}. \quad \text{then} \quad \overline{g}(x)_{ab} = H^A_a H^B_b G(X)_{AB}.$$

For $\mathbf{F} = D\Phi : T_X \mathfrak{B} \to T_x \mathcal{S}$, we have $\mathbf{F} = F_A^{\ a} e_a \otimes dX^A$, where $F_A^{\ a}(X) = \partial_A \Phi^a$ and its inverse $\Phi^*(x) : T_x \mathcal{S} \to T_X \mathfrak{B}$ is given by $\Phi^*(x) = Q_b^A(x) E_A \otimes dx^b$ where $Q_b^A(x) F_A^{\ a}(X) = \delta_b^a$. We have

$$\nabla_{\Phi^* e_b}(\Psi^{-1}e_a) = \nabla_{Q^A_b E_A}(H^B_a E_B) = Q^A_b(H^B_a \nabla_{E_A} E_B + \partial_A H^B_a E_B) = Q^A_b(H^B_a \Gamma^C_{AB} + \partial_A H^C_a)E_C.$$

Hence,

$$\overline{\nabla}_{e_b}e_a = \Psi(\nabla_{\Phi^*e_b}\Psi^{-1}e_a) = \Psi_C^{\ c}Q_b^A \Big(H_a^B\Gamma_{AB}^C + \partial_A H_a^C\Big)e_c.$$

Therefore, the connection coefficients are

$$\overline{\Gamma}^{c}_{\ ba} = \Psi^{\ c}_{C} Q^{A}_{\ b} \Big(H^{B}_{\ a} \Gamma^{C}_{AB} + \partial_{A} H^{C}_{\ a} \Big).$$
⁽⁵⁾

The torsion tensor of the connection is defined by $\overline{T}(u, v) = \overline{\nabla}_u v - \overline{\nabla}_v u - [u, v]$. In components,

$$\overline{T}^{a}_{\ bc} = \overline{\Gamma}^{a}_{\ bc} - \overline{\Gamma}^{a}_{\ cb}.$$
(6)

For holonomic transformation, this current torsion tensor is related to the torsion of the reference manifold as:

$$\overline{T}(u,v) = \overline{\nabla}_u v - \overline{\nabla}_v u - [u,v] = \Phi_*(\nabla_{\Phi^*u} \Phi^* v - \nabla_{\Phi^*v} \Phi^* u - [\Phi^* u, \Phi^* v]) = \Phi_* T(\Phi^* u, \Phi^* v).$$
(7)

Last the current curvature tensor is defined by $\overline{R}(u, v)w = \overline{\nabla}_u \overline{\nabla}_v w - \overline{\nabla}_v \overline{\nabla}_u w - \overline{\nabla}_{[u,v]} w$. Put $U = \Phi^* u$, $V = \Phi^* v$ and $W = \Psi^{-1} w$, we have the following relation

$$\overline{R}(u,v)w = \overline{\nabla}_u \Psi(\nabla_{\Phi^*v}\Psi^{-1}w) - \overline{\nabla}_v \Psi(\nabla_{\Phi^*u}\Psi^{-1}w) - \Psi(\nabla_{\Phi^*[u,v]}\Psi^{-1}w) = \Psi(\nabla_{\Phi^*u}\nabla_{\Phi^*v}\Psi^{-1}w - \nabla_{\Phi^*v}\nabla_{\Phi^*u}\Psi^{-1}w - \nabla_{[\Phi^*u,\Phi^*v]}\Psi^{-1}w) = \Psi R(U,V)W.$$
(8)

The curvature \overline{R} vanishes if and only if R is zero. Indeed, because det F > 0 and det $\Psi > 0$ then

vanishing \overline{R} means $\Psi R(U, V)W = 0$, $\forall V, U, W \in T\mathfrak{B}$. Then, R(U, V)W = 0, $\forall V, U, W \in T\mathfrak{B}$ hence R = 0.

For holonomic transformation ($ie \Psi = \mathbf{F}$) of a body without initial defect (ie R = 0, T = 0), we necessarily obtain $\overline{T} = 0$ and $\overline{R} = 0$. In other words no defects appears in the current state. Conversely, for nonholonomic transformation we have $\overline{R} = 0$, but $\overline{T} \neq 0$ ie. non-zero dislocation density. Physical meaning of this situation can be seen through a process for which micro-structure is not convected by the macro-scale transformation.

Remark 2.3. Let assume $\Phi(X) = x$, then $Q = \mathbb{I}$, besides, we also consider $\Gamma_{AB}^C = 0$. In that case there are no torsion and curvature on \mathfrak{B} , A priori the current connection has non-zero torsion while vanishing curvature. The connection coefficients on $\Phi(\mathfrak{B})$ are given by

$$\overline{\Gamma}^{c}_{\ ba} = \Psi^{\ c}_{C} \frac{\partial H^{C}_{\ a}}{\partial X^{A=b}} = -H^{C}_{\ a} \partial_{X^{b}} \Psi^{\ c}_{C}. \tag{9}$$

In general, a distribution of dislocations, leads to residual stresses essentially because the body is constrained to deform in Euclidean space. If one partitions the body into small pieces, each piece will individually relax, but it is impossible to realize a relaxed state for the whole body by combining these pieces in Euclidean space, that is, they does not fit together. Any attempt to reconstruct the body by sticking the particles together will induce deformations on them. The process of relaxation after the piece is cut corresponds to a linear deformation of this piece (linear, since the piece is small). Let us call this deformation F_p . The deformation gradient of the body at this piece F can be decomposed as $F = F_e F_p$, where, by definition, $F_e = F F_p^{-1}$. This process introduces an "intermediate" configuration. This intermediate configuration is not compatible and is understood as an auxiliary configuration defined locally. Has showed in [3] this intermediate configuration is not necessary: one can define a global stress-free reference manifold instead of working with local stress-free configurations by the fact that one can combine the reference and intermediate configurations into a parallelizable material manifold, in which F_p is defined as a moving frame on this manifold. In addition, the material manifold is endowed with an evolving connection (compatible with the metric) such that the non-coordinate basis is everywhere parallel. In such a way, the coefficients connection is given by $\Gamma^{I}_{JK} = (\mathbf{F}_{p}^{-1})^{I}_{\alpha}\partial_{J}(\mathbf{F}_{p})^{\alpha}_{K}$. This connection has non-zero torsion, but vanishing curvature. The new manifold is considered as the stress-free reference configuration. The connection and metric defined on it presents the distribution of dislocations on the initial state [3].

3 Strain Measures

Recall, the classical elastic strain tensor

$$\mathbf{E} = \frac{1}{2}(\Phi^* g - G). \tag{10}$$

A new strain, called the nonholonomic strain, is introduced in order to measure the difference between the motion of the point and frame. It is given by:

$$\mathcal{E} = (\Psi - \mathbf{F})^* g, \tag{11}$$

where $\mathcal{E}(U, V) = g((\Psi - \mathbf{F})U, (\Psi - \mathbf{F})V), \forall U, V \in T\mathfrak{B}$. In components, $\mathcal{E}_{AB} = (\Psi - \mathbf{F})^a_A (\Psi - \mathbf{F})^b_B g_{ab}$.

Proposition 3.1. The tensor \mathcal{E} is symmetric. It vanishes if and only if $\Psi = \mathbf{F}$. Moreover, \mathcal{E} is invariant under arbitrary body rotation \mathcal{Q} ie if $\hat{\Psi} = \mathcal{Q}\Psi$ and $\hat{\mathbf{F}} = \mathcal{Q}\mathbf{F}$, $\hat{\mathcal{E}} = \mathcal{E}_{,.}$

Proof. Of course, if $\Psi = \mathbf{F}$, $\mathcal{E} = 0$. Conversely, if $\mathcal{E} = 0$, we get $g((\Psi - \mathbf{F})V, (\Psi - \mathbf{F})V) = 0$, $\forall V \in T\mathfrak{B}$. Since g is the metric on \mathcal{S} , $(\Psi - \mathbf{F})V = 0$, $\forall V \in T\mathfrak{B}$, hence $(\Psi - \mathbf{F})_A^a = 0$ or $\Psi = \mathbf{F}$. Due to symmetry of g, the nonholonomic strain is symmetric. Finally we have $\hat{\mathcal{E}}(V, W) = g((\hat{\Psi} - \hat{\mathbf{F}})V, (\hat{\Psi} - \hat{\mathbf{F}})W) = g(\mathcal{Q}(\Psi - \mathbf{F})V, \mathcal{Q}(\Psi - \mathbf{F})W) = g((\Psi - \mathbf{F})V, \mathcal{Q}^T\mathcal{Q}(\Psi - \mathbf{F})W) = g((\Psi - \mathbf{F})V, (\Psi - \mathbf{F})W) = \mathcal{E}(V, W)$. Hence $\hat{\mathcal{E}} = \mathcal{E}$.

Let introduce the gliding angle $\Theta = \Theta^I E_I$ with $0 \le \Theta^I < \pi$ such that

$$\cos \Theta^{I} = \frac{\left|g(\Psi E_{I}, \mathbf{F} E_{I})\right|}{\sqrt{g(\Psi E_{I}, \Psi E_{I})}\sqrt{g(\mathbf{F} E_{I}, \mathbf{F} E_{I})}}.$$
(12)

Notice that if $\Psi = \mathbf{F}$, $\Theta = 0$, but the converse is not true, as an example for $\Psi = c\mathbf{F}$ with c > 0 we have $\Theta = 0$. The gliding angle can be rewritten as

$$2\cos\Theta^{I} = \frac{g(\Psi E_{I}, \Psi E_{I}) - \mathcal{E}(E_{I}, E_{I}) + g(\mathbf{F} E_{I}, \mathbf{F} E_{I})}{\sqrt{g(\Psi E_{I}, \Psi E_{I})}\sqrt{g(\mathbf{F} E_{I}, \mathbf{F} E_{I})}}.$$
(13)

Finally, the microscopic strain can be defined by

$$\underline{\mathbf{E}} = \frac{1}{2} (\Psi^* g - G), \tag{14}$$

where $\Psi^*g(U,V) = g(\Psi U,\Psi V), \forall U,V \in T\mathfrak{B}$. In components, $\underline{\mathbf{E}}_{AB} = \frac{1}{2}(g_{ab}\Psi^b_A\Psi^a_B - G_{AB}).$

Proposition 3.2. If $\Psi = QF$, where Q is a rotation, then $\underline{E} = E$.

Proof. We denote $g_x(u, v) = \langle u, v \rangle_x$, $\forall u, v \in T_x S$ and $G_X(U, V) = \langle U, V \rangle_X$, $\forall U, V \in T_X \mathfrak{B}$. Let $A : T_X \mathfrak{B} \to T_x S$ be a linear transformation. Then the transpose of A, written A^T , is the linear transformation $A^T : T_x S \to T_X \mathfrak{B}$ such that $\langle AW, v \rangle_x = \langle W, A^T v \rangle_X$, for all $W \in T_X \mathfrak{B}$ and $v \in T_x S$. For all $V, W \in T \mathfrak{B}$, we have $\Psi^* g(V, W) = \langle \Psi V, \Psi W \rangle_x = \langle Q \mathbf{F} V, Q \mathbf{F} W \rangle_x = \langle V, \mathbf{F}^T Q^T Q \mathbf{F} \rangle_X = \langle V, \mathbf{F}^T \mathbf{F} V \rangle_x = \langle \mathbf{F} V, \mathbf{F} W \rangle_X = \Phi^* g(V, W)$. Hence, $\mathbf{E} = \mathbf{E}$.

Physical interpretation: In this microcontinuum model, the body \mathfrak{B} is considered to be a collection of finite material particles $\{\mathbf{P}\}$. The mapping Φ may be seen as the motion of the centroid of the particle. Transformation of the microstructure is characterized along vectors \underline{V} attached to the particle and is identified by the mapping Ψ . Change of the distances between neighboring material point \mathbf{P} is measured by the classical elastic strain \mathbf{E} . This refers to the macro-stretching of the body caused by the motion Φ . The transformation of direction \underline{V} illustrates the change of the shape of the element, by using the microscopic strain.

As $\underline{\mathbf{E}}$ can be used to measure the micro-stretching of the body caused by the motion Ψ a total internal energy can be taken into the following form $\Xi(X) = \Xi_{\Phi}(\mathbf{E}, X) + \underline{\Xi}_{\Psi}(\underline{\mathbf{E}}, X)$, where $\Xi_{\Phi}, \underline{\Xi}_{\Psi}$ are the macrostructural energy (or macroscopic energy) and the microstructural energy respectively.

The incompatibility of the macro and micro motion is described by the nonholonomic strain \mathcal{E} . This leads to an energy function defined with an other point of view. Indeed the total internal energy can be written as $\Xi(X) = \Xi_{\Phi}(\mathbf{E}, X) + \Xi_{\Psi}(\mathcal{E}, X)$ too where $\Xi_{\Psi}(\mathcal{E}, X)$ is an other energy function depending on \mathcal{E} . If $\Psi = \mathbf{F}$, the microcontinuum model can be considered to be the macrocontinuum model. This situation can be observed by the second decomposition, but it is not the case in the first decomposition. For this reason, we privilege \mathcal{E} and the use the second decomposition $\Xi(X) = \Xi_{\Phi}(\mathbf{E}, X) + \Xi_{\Psi}(\mathcal{E}, X)$.

4 Example

Let consider an example where reference configuration is defined by R = 0 and T = 0, $g = \delta$; the motion Φ be identity, then $\mathbf{F} = \mathbf{Q} = \mathbb{I}$. Last we consider Ψ given as below

$$\Psi_B^a = \begin{pmatrix} 1 & \psi & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ then } H_a^B = \begin{pmatrix} 1 & -\psi & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
(15)

where $\psi: \mathfrak{B} \to \mathbb{R}$ is C^{∞} . The induced metric is $\overline{g}_{ab} = H^A_a H^B_b \delta_{AB} = H^A_a H^A_b$, and hence

$$\overline{g}_{ab} = \begin{pmatrix} 1 & -\psi & 0\\ -\psi & 1+\psi^2 & 0\\ 0 & 0 & 1 \end{pmatrix}.$$
 (16)

Of course the elastic strain **E** is zero. The non-zero coefficients of the nonholonomic strain are $\mathcal{E}_{22} = (\Psi - \mathbf{F})_2^{\ 1}(\Psi - \mathbf{F})_2^{\ 1}g_{11} = \psi^2$. The connection coefficients: $\overline{\Gamma}_{b2}^1 = \Psi_1^{\ 1}\frac{\partial H_2^1}{\partial X^{A=b}} = -\partial_{X^b}\psi$. This yields to non-vanishing torsion $\overline{T}_{\alpha 2}^1 = -\partial_{X^{\alpha}}\psi$ with $\alpha = \{1, 3\}$, in which \overline{T}_{32}^1 is screw-type dislocation and \overline{T}_{12}^1 is edge-type dislocation. In particular, if ψ depends only on X^1 , we obtain a edge-type dislocation density, whereas if ψ depends X^3 only, the new material contain after transformation a density of screw-type dislocation. Last if ψ is function of X^2 , the current state is defect free after transformation.

If $\psi(X^2)$, we have an interesting situation where the nonholonomic strain is not zero but torsion and curvature both vanishes. In other words, this example illustrate the following : for non-zero nonholonomic strain, the torsion and curvature is zero but the converse is not true.

References

- [1] E.Kröner. *Continuum theory of defects*. In R. Balian et al., editor, Less Houches, Session XXXV, 1980-Physics of defects. Amsterdam, North-Holland Publishing Company, 1981.
- [2] Jerrold E.Marsden and Thomas J.R. Hughes. *Mathematical Foundations of Elasticity*. Dover, New York, 1983.
- [3] A.Yavari and A.Goriely, "*Riemann-Cartan Geometry of Nonlinear Dislocation Mechanics*". Archive for Rational Mechanics and Analysis 205.1 (2012). Doi: 10.1007/s00205-012-0500-0.