

Non-Euclidean Structures as Internal Variables in Non-Equilibrium Thermomechanics

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**Dedicated to the Memory of Grigorios TSAGAS (1935-2003),
President of Balkan Society of Geometers (1997-2003)**

Abstract

We reconsider from a geometrical viewpoint the model of continuum thermodynamics which includes a non-Euclidean metric in an intermediate configuration as an internal variable of thermomechanical origin. We investigate the deep relations existing between such a choice of an internal variable and a microstructure approach in which the order parameter is a triad of vectors orthonormal in the internal metric.

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1 Introduction

In a recent paper [1] one of us (V.C.) together with other authors has investigated properties and relationships between a macroscopic and a microscopic (or *internal*) metric variable in the context of thermodynamics for visco-anelastic media. The purpose of this paper is to further discuss the possible existence of such an internal metric among a possibly larger set of internal variables, by adopting a geometrical view based on the bundle theoretical framework for continuum thermomechanics and, in particular, on the modern perspective about Cartan's *moving frame technique*.

Reasons for introducing a metric among the internal variables which the description of thermodynamics in a continuous medium may need or suggest are manifold. This is due to a number of reasons, among which the main one seems to be related with the process of model approximation of a body (an inhomogeneous aggregate of small portions with possibly different physical properties) which is thought as a truly continuous body formed by material points (having, of course, just a virtual meaning). Most materials existing in nature (crystals, granular bodies, etc..) should in fact admit a description at a *mesoscopic level* (see e.g. [2],[3] and references quoted therein) in which each single portion is analyzed in detail. Since such a detailed analysis is in fact practically impossible the only viable solution is to hide in a suitable parameter

space (such as a set of internal variables [4],[5],[6],[7],[8] or the *mesoscopic space* of [2]) all the information which at each single point of the modelling body encodes, in fact, the mutual relations of a mesoscopic cell surrounding the chosen point with all the neighboring mesoscopic cells (or *grains*) of the true medium. Having assumed that the true body is embedded in our Euclidean 3-dimensional space (or in space-time whenever a relativistic description is envisaged) this information will be summarized by a number of scalar, vector and tensor fields on the modelling body which will be considered as a suitable set of *internal variables* suggested by a particular modellization of the physical phenomena under consideration.

In particular, different reasons may lead one to introduce a (generally non-Euclidean) metric among the internal variables of a body. As we shall shortly see later, this may have to do with purely mechanical properties of the body if it is assumed to have a *microstructure* (see [9],[10]), i.e. whence a framework à la Cosserat [11] is chosen. Another more stringent reason comes from the possibility that a *local internal metric* be induced by the atomic (or molecular, or granular) structure of the medium, here including also thermodynamical effects far from equilibrium, such as voids, inclusions and dislocations which realize a conceptual connection between the micromotion and the global material behavior (see, e.g. [12],[13],[14],[15]).

Following [1], we adopt the view that true media are described as *hypercontinua*.

We call *hypercontinuum* a material domain which is an aggregate of discrete *microscopic subdomains*, the nature of which depends on the observational scale, e.g. a granular material which may be viewed as made of grains, [14]. If the microscopic subdomains are too small to be detected only the motion of certain aggregates of microscopic subdomains can be observed and these detectable subsets will be called *mesoscopic subdomains* [16],[17]. Along a thermodynamical process the individual microdomains may migrate and diffuse, so that a domain's neighbour is constantly changing [18]. This micromotion may influence the topology of the body, resulting thus in a (non-affine) deformation superposed on the deformation of a mesodomain giving rise to a possible and generally non-Euclidean local structure.

Because of these one is therefore led to choose a (non-Euclidean) local metric among the internal variables. This metric should take into account the non-reversibility of thermodynamical processes occurring in the continuum (in particular dissipative phenomena), thus leading to extra terms in the Clausius-Duhem inequality (see [19],[20] and eqn. (4.3) of [1]) and in an effective entropy production (see, e.g. eq.n (4.9) of [1]). For other possible relations between thermodynamics and the existence of an internal metric we refer the reader to [15] (and ref.s quoted therein).

Since the modelling body is embedded into Euclidean space \mathbf{R}^3 (or, possibly, into a more complicated ambient space endowed with a pre-assigned or dynamical metric structure) the body \mathcal{B} is also endowed from the very beginning with an *ambient metric* which has to do with its purely mechanical behaviour. Even if these two metrics have a completely different physical origin and meaning, still they both exist at each single point of the body, so that it is meaningful to investigate their possible mathematical interrelationship. This justifies the contents of section 2 of [1], which we shall shortly review in this paper.

The interested reader may find a different interesting perspective on the geometry of triads as order parameters in the relatively recent paper by Magin [27]

2 The thermomechanical model

In [1] the following model was used to investigate the dynamics of a continuum with internal variables. The abstract body is a 3-dimensional manifold \mathcal{B} which, if necessary, might be considered to be from the beginning a subset of Euclidean space (\mathbf{R}^3, e) , where e denotes the Euclidean metric which in global Cartesian coordinates X^L ($L = 1, 2, 3$) reads as follows:

$$(2.1) \quad e = \delta_{LM} dX^L \otimes dX^M.$$

A configuration of the body is an embedding $\varphi : \mathcal{B} \rightarrow \mathbf{R}^3$ (definitions and notations of differential geometry are standard; we refer the reader to [21], [22], [23]). The *motion* of the body is a sufficiently regular curve of such embeddings $\varphi_t, t \in I \subseteq \mathbf{R}$, i.e. a regular succession of instantaneous configurations. Whenever an initial *reference configuration* $\varphi : \mathcal{B} \rightarrow \mathbf{R}^3$ is chosen (notice that by no means it is necessary to assume that φ is one of the motion configurations) the motion φ_t induces diffeomorphisms $\chi_t : \varphi(\mathcal{B}) \rightarrow \varphi_t(\mathcal{B})$ according to the rule:

$$(2.2) \quad \chi_t = \varphi_t \circ \varphi^{-1}$$

which provides the Lagrangian description of the body motion itself ¹. By an abuse of language we denote by $\mathcal{C} = \varphi(\mathcal{B})$ the *reference configuration* and by $\mathcal{C}_t = \varphi_t(\mathcal{B}) = \chi_t(\mathcal{C})$ the *actual configuration* (see Fig. 1).

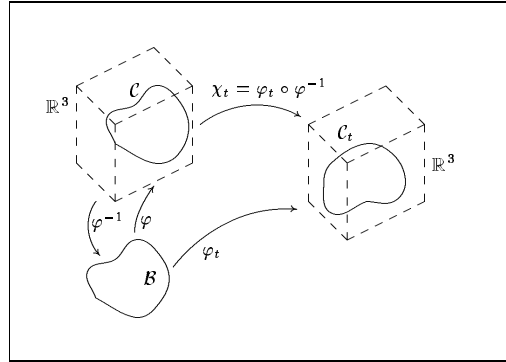


Figure 1: φ is the reference configuration, φ_t the motion and χ_t the Lagrangian description of motion.

Fig. 1

Following an idea which is sometimes useful in the modellization of continua (see, e.g., [24],[25] or [26] in a different context) it was assumed in [1] that besides the reference configuration $\mathcal{C}_0 \equiv \mathcal{C}$ and the actual configuration \mathcal{C}_t a third *intermediate* configuration $\tilde{\mathcal{C}}_t$ has to be assigned a physical meaning (in fact, one at each instant of time).

The reference (or initial configuration) \mathcal{C} is assumed to have the standard Euclidean structure induced by the ambient space. The deformation z_t from $\tilde{\mathcal{C}}_t$ to \mathcal{C}_t is the typical diffeomorphism of classical continuum mechanics, while the deformation $\psi_t = z_t^{-1} \circ \chi_t$

¹Being φ an embedding the inverse $\varphi^{-1} : \varphi(\mathcal{B}) \rightarrow \mathcal{B}$ is well defined and it is a diffeomorphism.

from \mathcal{C}_0 to $\tilde{\mathcal{C}}_t$ is more general, since it accounts for the deformation of the non-Euclidean structure induced by mesoscopic phenomena. The situation is described by Fig. 2.

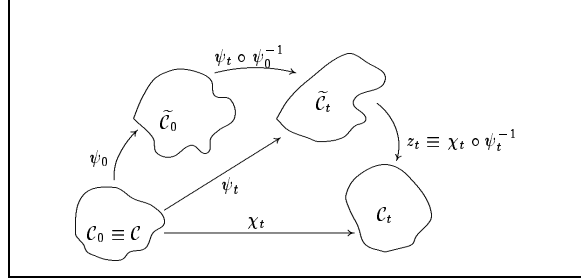


Figure 2: **The dynamic intermediate configurations.** Being χ_t the motion, ψ_0 defines the "reference intermediate configuration" so that ψ_t (or equivalently $\psi_t \circ \psi_0^{-1}$, accounts for the evolution of the internal variables.

Fig. 2

Let us now fix an instant of time t_* and consider, as in [1], the three configurations \mathcal{C}_0 , $\mathcal{C}_* = \tilde{\mathcal{C}}_{t_*}$ and \mathcal{C}_t . Denoting by \mathbf{e}_L ($L = 1, 2, 3$) an orthonormal basis of (\mathbf{R}^3, e) , where the body is initially embedded, the position of points of \mathcal{C}_0 will be denoted by vectors $\mathbf{X} = X^L \mathbf{e}_L$, where X^L are Cartesian coordinates (in \mathbf{R}^3 and thus in \mathcal{C}). In [1] the following (local) notation is introduced. The vector position of points in \mathcal{C}_* is denoted by

$$(2.3) \quad \boldsymbol{\xi} = \chi(\mathbf{x}, t_*) = \xi^\alpha \mathbf{e}_\alpha, \quad (\alpha = 1, 2, 3),$$

ξ^α being local coordinates in \mathcal{C}_* (and having tacitly assumed $\mathbf{e}_\alpha = \partial/\partial\xi^\alpha$). The motion (which in our current notation is $z_{t_*} = \chi_t \circ \psi_{t_*}^{-1}$) for any $t > t_*$ is represented by a function $\chi_*(\boldsymbol{\xi}, t)$ which maps \mathcal{C}_* into \mathcal{C}_t . The position of the points of \mathcal{C}_t is identified by:

$$(2.4) \quad \mathbf{x} = \chi_*(\boldsymbol{\xi}, t) = x^i \mathbf{e}_i, \quad (i = 1, 2, 3),$$

where (local) coordinates x^i are chosen in \mathcal{C}_t (again having tacitly assumed $\mathbf{e}_i = \partial/\partial x^i$). Moreover, the following notation is also adopted in [1]: the *deformation tensor* from \mathcal{C} to \mathcal{C}_* is denoted by Φ_L^α , while the *deformation gradient* from \mathcal{C}_* to \mathcal{C}_t is obviously given by $F_\alpha^i \equiv \partial x^i / \partial \xi^\alpha$. The following (local) objects are defined in [1]:

$$(2.5) \quad C_{LM} = C_{\alpha\beta} \Phi_L^\alpha \Phi_M^\beta$$

where

$$(2.6) \quad C_{\alpha\beta} = \delta_{ij} F_\alpha^i F_\beta^j$$

is the right Cauchy-Green deformation tensor relative to the deformation from \mathcal{C}_* to \mathcal{C}_t ;

$$(2.7) \quad B^{ij} = F_\alpha^i F_\beta^j g^{\alpha\beta}$$

where $\|g^{\alpha\beta}\| = \|g_{\alpha\beta}\|^{-1}$ is the contravariant metric tensor of the intermediate configuration \mathcal{C}_* induced by mesoscopic phenomena (i.e. $ds_*^2 = g_{\alpha\beta} d\xi^\alpha \otimes d\xi^\beta$). Notice that one is explicitly assuming that the standard Euclidean metric is again used in \mathcal{C}_t

to define $C_{\alpha\beta}$ as in (2.6) and that B^{ij} is the inverse of the *Finger tensor* relative to the deformation from \mathcal{C}_0 to \mathcal{C}_t , namely:

$$(2.8) \quad c_{ij} = g_{\alpha\beta} F_i^\alpha F_j^\beta$$

being $\| F_i^\alpha \| = \| F_\alpha^i \|^{-1}$. According to this (local) notation the Euclidean metric of \mathcal{C}_0 is

$$(2.9) \quad ds_0^2 = \delta_{LM} dx^L \otimes dx^M = g_{\alpha\beta} d\xi^\alpha \otimes d\xi^\beta$$

(the last being, in fact, the pull-back onto \mathcal{C}_* by means of ψ_t), having set

$$(2.10) \quad g_{\alpha\beta} = \delta_{LM} \Phi_\alpha^L \Phi_\beta^M$$

where $\| \Phi_\alpha^L \| = \| \Phi_L^\alpha \|^{-1}$.

Analogously one has also:

$$(2.11) \quad ds_0^2 = \delta_{LM} dx^L \otimes dx^M = c_{ij} dx^i \otimes dx^j$$

(the last being, in fact, the pull-back onto \mathcal{C}_t by means of χ_t), having defined c_{ij} according to (2.8). The inverse of (2.10) is obviously the following:

$$(2.12) \quad g^{\alpha\beta} = \delta^{LM} \Phi_L^\alpha \Phi_M^\beta.$$

These equations correspond to eqn.s (2.3)-(2.12) of [1].

In [1] a number of geometric propositions are proven about the invariants of the three metrics C_{LM} , B^{ij} and

$$(2.13) \quad g^{LM} = \delta^{\alpha\beta} \Phi_\alpha^L \Phi_\beta^M.$$

3 Continua with microstructure and metrics revisited

Our next aim will be to exploit the geometrical meaning of all the local formulae and results of [1] we shortly reviewed in section 2. Before doing this we have first to shortly comment about the geometrical formulation of *continua with a microstructure* and about a method which is commonly used in relativistic theories after Cartan's ideas of "moving frames".

Following [9] a *continuum with microstructure* consists of a body \mathcal{B} for which a regular manifold \mathcal{M} is assigned, the points of which (denoted by ν) represent a microstructural conditions (*order parameter*). A transformation group is defined on \mathcal{M} to account for the effects of (local) rotations onto the *order parameters* of the theory, so that for any $\nu \in \mathcal{M}$ and any rotation $Q \in SO(3)$ – the orthogonal group of the Euclidean space (\mathbf{R}^3, e) – there exists a unique representant $\nu_{(q)} \in \mathcal{M}$.

Moreover, there is a class \mathcal{U} of mappings $\mathcal{B} \rightarrow \mathbf{R}^3 \times \mathcal{M}$ denoted by $X \mapsto (\chi(X), \nu(X))$, called *complete positions*, such that the following axioms hold:

- i) the apparent position $\chi(X)$ is an injective mapping $\mathcal{B} \rightarrow \mathbf{R}^3$;
- ii) every pair (χ', χ'') of apparent positions is such that the bijection from $\mathcal{B}' = \chi'(\mathcal{B})$ onto $\mathcal{B}'' = \chi''(\mathcal{B})$ is regular ;

- iii) each complete position (χ, ν) is such that $\nu \circ \chi^{-1}$ from \mathcal{B} to \mathcal{M} is regular ;
- iv) if $(\chi, \nu) \in \mathcal{U}$ and $Q \in SO(3)$, then also $(\xi_{(q)}, \nu(q))$ belongs to \mathcal{U} , being $\chi_{(q)} = Q \circ \chi$ the effect of the rotation Q onto the vectors of \mathbf{R}^3 defined by $\chi : \mathcal{B} \rightarrow \mathbf{R}^{32}$.

Based on this heuristic definition a geometrical description of microstructures in continua may be given in a bundle-theoretic language by assuming the existence of a suitable bundle over the body having as fiber an appropriate sub-group of the orthogonal group $SO(3)$, the choice of which is dictated by the model, so that this principal bundle replaces \mathcal{B} as configuration space for the theory (see, e.g. [28], [29]). Here we are not interested into this possibility, which is beyond the scopes of this paper, but we have recalled this in order to mention that the assumption about the existence of "order parameters" controlled by (subgroups of) the orthogonal group $SO(3)$ is in fact equivalent to state that a number of phenomena of mechanical origin (and related to the choices of some preferred vectors and/or directions at each point of the body) is in fact a choice of suitable "internal variables" (in the sense of [4], [5]) which, instead of being thermodynamical, are purely mechanical and in fact related to a metric (the Euclidean metric of the ambient space). This viewpoint is coherent also with the so-called "mesoscopic descriptions" of continua in the sense of [17].

The approach of [15] and [1] is, mathematically speaking, a modellization of the same kind, although this time the internal variable *is* (and it is not simply *related to*) a metric, and moreover this metric does not account for local rotational degrees of freedom of mechanical origin but rather for local deformation properties of mesoscopic domains, which reflect into deviations from the Euclidean behavior.

Why do we come again to discuss this framework? The purpose is to make explicit the relation between the formalism developed in [1] and the *moving frame* technique of Cartan (see [30]) which, in fact, is at the basis of the modern perspective on the dynamics of Cosserat continua (see [11], [29]).

To this purpose, let us first consider the meaning of the *deformation tensor* Φ_L^μ introduced in section 2, which (according to the general theory; see, e.g. [1], [24]), being responsible of microlocal changes in the material, is assumed not to be a Jacobian. Let us refer to Fig. 3, where $\psi_t : \mathcal{C} \rightarrow \mathcal{C}_*$ is the deformation from the Euclidean configuration (\mathcal{C}, e) to the non-Euclidean configuration (\mathcal{C}_*, g) . By an abuse of notation we denote by e also the metric induced by the Euclidean metric of \mathbf{R}^3 onto the embedded $\mathcal{C} \subseteq \mathbf{R}^3$.

As before, let X^L be local (Eulerian) coordinates in \mathcal{C} and let ξ^α be local coordinates in \mathcal{C}_* around any image point under consideration. Then Φ defines, for each $X \in \mathcal{C}$, a linear map from the tangent space $T_X \mathcal{C}$ to the tangent space $T_p \mathcal{C}_*$, $p = \Phi(X)$, by the rule:

$$(3.1) \quad \mathbf{u} = u^L \mathbf{e}_L \mapsto (\Phi_L^\mu u^L) \partial_\mu \in T_p \mathcal{C}_* .$$

Assuming that Φ is not the Jacobian of the transformation ψ_t , which is locally represented by equations $\xi^\alpha = \psi^\alpha(t, X)$, amounts to state that $\Phi_L^\mu \neq \partial \xi^\alpha / \partial X^L$, which in intrinsic notation means the following:

²Notice that this definition is fully coherent, via a slight abuse of language, with the previous notation, being X a configuration in \mathcal{B} , which we consider to be already embedded into \mathbf{R}^3 by means of the initial configuration φ of section 1, while lower case letters x denote the actual configuration of \mathcal{C}_t

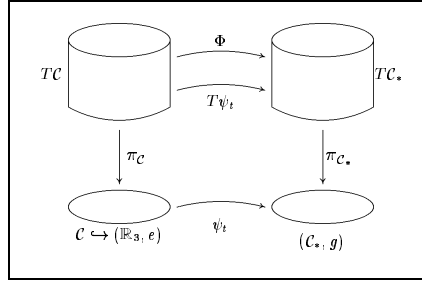


Figure 3: The geometrical meaning of the deformation tensor Φ .

Fig. 3

$$(3.2) \quad \Phi \neq T\psi_t$$

being $T\psi_t : TC \rightarrow TC_*$ the tangent map of ψ_t between the tangent bundles (see [21]). Therefore, we see that imposing a non-Jacobian deformation Φ_L^μ amounts to choose a linear bundle map $\Phi : TC \rightarrow TC_*$ which transports vectors but it is not the standard pull-back map (i.e., the tangent map). According to a slightly different perspective, the map Φ defines a tensor field of rank $(1, 1)$. Considering as fixed the Cartesian coordinates (i.e., leaving indices L unchanged) the components Φ_L^μ transform as vectors in \mathcal{C}_* , so that:

$$(3.3) \quad \mathbf{E}_L \equiv (\Phi_L^\mu) \partial_\mu$$

is a non-holonomic base for each $T_p\mathcal{C}_*$. The triple $\{\mathbf{E}_L\}$ ($L = 1, 2, 3$) is therefore a moving frame in the sense of Cartan (which is non-holonomic since Φ is not a Jacobian).

Recall now the existence of a global bundle identification (is any preferred signature) between the space of metrics in any manifold \mathcal{M} and the space of tensorfields $T_1^1(\mathcal{M})$ (see, e.g., [31] page 154, [32], [33] and refs. quoted therein). Locally it is given by:

$$(3.4) \quad g_{\mu\nu} = \eta_{ab} e_\mu^a e_\nu^b \quad (\mu, \nu = 1, \dots, n; a, b = 1, \dots, n),$$

where $n = \dim(\mathcal{M})$ and η is the given signature, i.e. the diagonal matrix $\eta = (+1, \dots, +1, -1, \dots, -1)$; e_μ^a is the $(1-1)$ tensorfield which locally represents a linear frame $\mathbf{e}_a = e_a^\mu \partial_\mu$.

The method of replacing a metric g in \mathcal{M} with a frame in the linear frame bundle $\mathbf{L}(\mathcal{M})$ is nothing but the origin of Cartan's technique, which is frequently used in Relativity (whereby $n = 4$ and the frame is often called a *tetrad*).

In our case $n = 3$ and (3.3) defines a *triad*. Then we easily see that the situation described in [1] is reflected in Fig. 4.

Passing from the initial configuration \mathcal{C} to the actual configuration \mathcal{C}_t through an intermediate configuration \mathcal{C}_* is a motion χ_t which is the composition of a motion $z_t : \mathcal{C}_* \rightarrow \mathcal{C}_t$, locally represented by (2.4), and a deformation $\psi_t : \mathcal{C} \rightarrow \mathcal{C}_*$, locally represented by (2.3). When acting on tangent vectors $\mathbf{u} \in TC$, the deformation gradient Φ transforms objects according to the rule (2.3), while the tangent map $Tz_t : TC_* \rightarrow \mathcal{C}_t$ transforms vectors by standard pull-back, i.e. the transformation matrix is the Jacobian of z_t , i.e. nothing but the *gradient of deformation*:

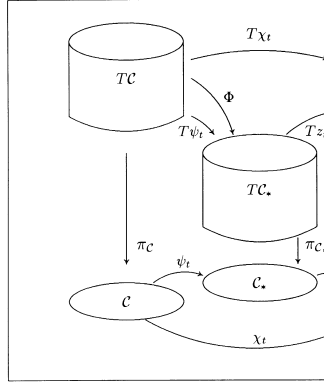


Figure 4: The deformation maps on vec

Fig. 4

$$(3.5) \quad F_{\alpha}^i \equiv \frac{\partial x^i}{\partial \xi^{\alpha}}$$

as correctly assumed in eqn. (2.2) of [1]. Of course this enters the definition of the right Cauchy-Green tensor as in our eqn. (2.6). In other words vectors will be finally transformed by the (non pull-back) local rule:

$$(3.6) \quad u^L e_L \mapsto (F_{\alpha}^i \Phi_L^{\alpha} u^L) \partial_i \in TC_t$$

which in intrinsic language is the bundle morphism

$$(3.7) \quad Tz_t \circ \Phi : TC \rightarrow TC_t$$

differing from the tangent map $T\chi_t = Tz_t \circ T\psi_t$ because of our assumption (3.2). Notice that (3.6) amounts to have decomposed the total deformation tensor into the product of the deformation $\|\Phi_L^{\alpha}\|$ with the gradient of deformation $\|F_{\alpha}^i\|$ as usually done when considering non-reversible composed transformations.

Basing ourselves on (3.6) or (3.7) we can now easily recover the local relations derived in [1], i.e. the equations which we have reported here as eqns. (2.5)–(2.13). It is an easy task for the reader to check that they amount to the following pair of equivalent algebraic relations:

$$(3.8) \quad g(\Phi(\mathbf{u}), \Phi(\mathbf{v})) = e(\mathbf{u}, \mathbf{v})$$

$$(3.9) \quad g(\mathbf{U}, \mathbf{V}) = e(\Phi^{-1}(\mathbf{U}), \Phi^{-1}(\mathbf{V})),$$

whereby: e is the Euclidean metric of \mathcal{C} ; g is the internal metric of \mathcal{C}_* ; \mathbf{u}, \mathbf{v} are vectors in \mathcal{C} and \mathbf{U}, \mathbf{V} are vectors in \mathcal{C}_* . Analogously for the transition from (\mathcal{C}_*, g) to (\mathcal{C}_t, e) , again Euclidean, which we leave to the reader. The above relations (3.8) and (3.9) fully justify theorems 2.1 and 2.2 of [1].

4 Conclusions

In conclusion, we have seen that assuming an intermediate configuration \mathcal{C}_* with a non-Euclidean metric g (of mesoscopic origin) and choosing a non-Jacobian deformation tensor $\Phi = \|\Phi_L^\alpha\|$ in the transformation rules (as, e.g. eqn. (3.6)), is equivalent to assume the existence of a dynamical triad \mathbf{E}_L as defined by (3.3).

In other words, the idea of choosing a non-Euclidean metric g as a tensorial internal variable (in the sense of [4],[5],[7]), which is ultimately related with the mesoscopic processes (in the sense of [2]) associated with dissipation and non-equilibrium thermodynamics, can be interpreted as the construction of a theory of micropolar continua à la Cosserat (in the sense of [9]) where the micropolar variable (i.e. the order parameter) is a *full* triad of vectors \mathbf{E}_L (without any a priori specific symmetry or condition) which, instead of having a mechanical origin has a thermomechanical genesis. This triad is not orthonormal with respect to the Euclidean body metric \mathbf{e} but reflects, instead, properties of the inner metric g ; they are, in fact, an orthonormal triad with respect to g , i.e. $g(\mathbf{E}_L, \mathbf{E}_M) = \delta_{LM}$, according to our eqn. (2.10) or, equivalently, to eqn. (2.7) of [1].

Some physical consequences of the introduction of a non-Euclidean metric g in the case of thermoelasticity of solids with visco-anelastic properties can be found in the original paper [1].

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