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Continuum Mechanics — *On Professor Grioli's last riddle: What boundary and initial conditions make sense for microstructured continua?*, by Paolo Podio-Guidugli, communicated on November 10, 2017.

In memory of Professor Giuseppe Grioli

Abstract. — An abridged but faithful exposition of Professor Grioli's version of the theory of microstructured continua of Cosserat type is given, so as to reformulate and discuss the title question. This exposition prompts some reflections on how to bridge by the use of continuum theories the gap between microscopic and macroscopic mathematical descriptions of matter.

Key words: Microstructured continua, initial/boundary conditions, Cosserat continua

Mathematics Subject Classification: 74Axx, 65Bxx

1. Introduction

In [1], his last journal papers appeared in 2003, Professor Giuseppe Grioli offered his own answer to a riddle that he had repeatedly proposed to the attention of the continuum mechanics community (see the literature quoted in [1], especially [2]). Here is how he makes his case in the introduction of [1].

To begin with, he spells out the difficulties he has with the standard theories of microstructured continua.

"As is well known, Cauchy's field and boundary equations, together with the initial conditions, are at the basis of Continuum Mechanics. Nevertheless, they are not sufficient for the study of many questions. More complex mathematical models are necessary, such as microstructures and, in particular, Cosserat's theory. But the analytical problem of microstructures demands more numerous data on the boundary and in the initial instant than Cauchy's theory. This is a very important point. In my opinion, it is in general very difficult to express the action that the external world exerts on a body through its boundary by means of physically significant known functions of its points, unlike what happens in the classical theory of Cauchy. For example, in Cosserat's microstructures it is necessary to give on the boundary the distribution of the external couples or, alternatively, some surface constraints, for example, to specify the local rotations.

In my opinion, the inconvenience is due to the procedure for setting the general equations, because it requires the introduction of concepts of dubious physical meaning as couple stress, hyperstress and so on. Consequently, according to the action-and-reaction principle, this would mean the attribution of special properties to the external world. I think that it is very difficult (indeed impossible) to give concrete examples in which the external couples due to the external world are known on the boundary. I think that the microstructure theory must be assumed to be a refinement of the classical theory of Cauchy, and that physical meaning must be given only to the traditional Cauchy stress, possibly not symmetric.''

He then delineates how those difficulties can be radically removed.

''The mathematical model of a microstructure must be obtained using as little as possible the concept of force, whose physical definition, according to Hertz ideas, is very difficult. This happens especially for internal forces and on the boundary. On the contrary, it is easier and more significant to operate starting from the mathematical concept of deformation, keeping in mind the corpuscular hypothesis on the matter of modern Physics.

I will show that it is possible to invent a theory of the microstructures that on the boundary demands only the knowledge of the data required by the classical Cauchy theory. The same happens for the initial conditions in the evolutive problems. Therefore, the microstructure's mathematical model will appear as a refinement of Cauchy theory, that must be considered as the general basis of all Continuum Mechanics.''

I have a couple of considerations to offer, prompted by the above quoted passages.

Firstly, Grioli's concern for 'physically significant' body-environment interactions points to situations where a mathematically consistent theory is tested experimentally for an ultimate indispensable validation of its predictions. Now, mathematically legal boundary conditions, both 'hard' and 'soft', may be difficult to realise in the laboratory, even when the adopted model is Cauchy's. If, for example, certain theoretically prescribable point-wise boundary displacements turn out difficult to induce in practice, one might be tempted to replace them by looser, and hence easier to realise, *confinement conditions*. But, such a measure would most probably entail unsurmountable analytic difficulties in establishing, say, the well-posedness of the modified mathematical problem. Secondly, it seems to me that Grioli's preoccupations with conventional models of microstructured continua had and have the merit, among others, to point out the need of making explicit the modeler's scale-bridging choices.

This paper is a late follow-up of an invited talk with identical title I gave during the conference ''New Frontiers in Continuum Mechanics'', held in Rome on June 21–22, 2016, at the Accademia Nazionale dei Lincei. In Section 2, I recapitulate briefly how Grioli solved his own modelling riddle. Then, in Section 3, I elaborate on the subject, in the light of some reflections on how to bridge the gap between microscopic and macroscopic mathematical descriptions of matter.

2. Grioli's argument

I hereafter give an abridged but faithful exposition of the argument offered by Grioli in [2] and, with more detail, in [1], in order to show that 'microstructures [should be seen] as a refinement of Cauchy theory'. For easier reference, I use a notation as close to his as possible for most of the objects that have central importance in his developments, e.g., for the referential and current position vectors of material points and for the stress measures; however, on indulging to an idiosyncrasy of mine and contrary to what he did, I make no use of Cartesian coordinates.

2.1. Deformation

Grioli denotes by C and C' the reference and current configurations of a three-dimensional continuous body; he also denotes by C'' a varied configuration 'very close to C''. In his views, in the case of a microstructured material body of Cosserat type, the matter comprising C consists of *sizeable elementary particles*, modeled as rigid bodies of diameter h, whose placement in the reference space is specified by a (mass center, rotation) pair $(G, \boldsymbol{R})$ and whose typical point is denoted by P. Points and particles in the current and varied configurations are decorated by superscript primes, one or two, respectively.

In a deformation of C into C', the *displacement* of P is $\boldsymbol{u} = PP'$: the *deformation gradient* is denoted by $\boldsymbol{F}$; the deformation measure is Cauchy–Green's:

$$\tilde{\boldsymbol{E}} = 1/2(\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{F}).$$

For c and c_1 two elementary particles respectively centred at G and G_1, and for $P \in c$ and $P_1 \in c_1$, let

$$GP =: \eta =: h\tilde{\eta}, \quad G_1P_1 =: \eta_1 =: h\tilde{\eta}_1 \quad \text{and} \quad GG_1 =: \xi,$$

so that

$$PP_1 = -\eta + \xi + \eta_1 = \xi + h(\tilde{\eta}_1 - \tilde{\eta});$$

the *dilatation coefficient* δ at point P in the direction of PP_1 is:

$$(1+\delta)^2(P, PP_1) := \frac{|P'P_1'|^2}{|PP_1|^2}.$$

Implicitly in [1] and explicitly in [2], Grioli assumes that $|\xi| > 0$ whatever the value of the scale parameter h; again more or less explicitly, he suggests that the kinematics of Cauchy continua is recovered in the $(h \to 0)$-limit, in the sense that both

$$\lim_{h\to 0} PP_1 = GG_1$$

and

$$\lim_{h\to 0}(1+\delta)^2(P, PP_1) = (1+\delta)^2(G, GG_1)$$
$$= \boldsymbol{F}^T(G)\boldsymbol{F}(G) \cdot \frac{\xi}{|\xi|} \otimes \frac{\xi}{|\xi|} = (\boldsymbol{1} - 2\tilde{E}(G)) \cdot \frac{\xi}{|\xi|} \otimes \frac{\xi}{|\xi|}.$$

Here is the supporting argument he sketches. Given that

$$P'P_1' = G'G_1' - G'P' + G_1'P_1',$$

he sets:

$$G'G_1' = \boldsymbol{F}\xi, \quad G'P' = \boldsymbol{R}\eta = h(\boldsymbol{R}\tilde{\eta}), \quad G_1'P_1' = \boldsymbol{R}_1\eta_1 = h(\boldsymbol{R}_1\tilde{\eta}_1),$$

so that

$$P'P_1' = \boldsymbol{F}\xi + h(\boldsymbol{R}_1\tilde{\eta}_1 - \boldsymbol{R}\tilde{\eta}),$$

and hence, as an easy computation shows,

$$(1+\delta)^2(P, PP_1) = (1+\delta)^2(G, GG_1) + O(h).$$

2.2. Balance laws

The basic balance laws are given by Grioli the following point-wise expressions:

In C,

$$\text{(1)} \qquad \mathrm{Div}(\boldsymbol{F}\tilde{\boldsymbol{T}}) + \boldsymbol{d}_f = \boldsymbol{0}, \quad \mathrm{Div}(\boldsymbol{F}\tilde{\boldsymbol{P}}) + \mathbb{e}[\boldsymbol{F}\tilde{\boldsymbol{T}}\boldsymbol{F}^T] + \boldsymbol{d}_c = \boldsymbol{0};$$

In ∂C, the boundary of region C,

$$\text{(2)} \qquad \boldsymbol{F}\tilde{\boldsymbol{T}}\boldsymbol{n} = \boldsymbol{c}_f, \quad \boldsymbol{F}\tilde{\boldsymbol{P}}\boldsymbol{n} = \boldsymbol{c}_c.$$

Here $\tilde{\boldsymbol{T}}$ is the *Cosserat stress* and $\tilde{\boldsymbol{P}}$ is the *couple stress*, two second-order tensors; the vectors $\boldsymbol{d}_f$, $\boldsymbol{d}_c$ and $\boldsymbol{c}_f$, $\boldsymbol{c}_c$ denote, respectively, volume and area densities of distance and contact forces and couples; $\mathbb{e}$ is the Ricci symbol, whose representation in terms of the three orthonormal vectors $\boldsymbol{e}_i$ is:

$$\mathbb{e} := \boldsymbol{e}_i \otimes \boldsymbol{W}_i, \quad \boldsymbol{W}_i = -\boldsymbol{e}_{i+1} \otimes \boldsymbol{e}_{i+2} + \boldsymbol{e}_{i+2} \otimes \boldsymbol{e}_{i+1} \quad (\textit{modulo } 3, \text{ no sum}),$$

whence

$$\mathbb{e}[\boldsymbol{A}] = (\boldsymbol{W}_i \cdot \boldsymbol{A})\boldsymbol{e}_i = (\boldsymbol{W}_i \cdot \mathrm{skw}\, \boldsymbol{A})\boldsymbol{e}_i;$$

equation $(1)_2$ can be equivalently written as

$$\text{(3)} \qquad \mathrm{Div}(\boldsymbol{F}\tilde{\boldsymbol{P}}) + \mathbb{e}[\boldsymbol{F}(\mathrm{skw}\, \tilde{\boldsymbol{T}})\boldsymbol{F}^T] + \boldsymbol{d}_c = \boldsymbol{0} \quad \text{in } C.$$

Recall that the Cosserat stress $\tilde{\boldsymbol{T}}$ is symmetric if and only if the Cauchy stress $\boldsymbol{T}$ is, because $\boldsymbol{T} := (\det \boldsymbol{F})^{-1}\boldsymbol{F}\tilde{\boldsymbol{T}}\boldsymbol{F}^T$; and that $\boldsymbol{F}\tilde{\boldsymbol{T}}$ is the stress measure introduced by Piola.

Systems $(1)_1$-$(2)_1$ and (3)-$(2)_2$ correspond, respectively, to systems (39) and (40) in [1].

2.3. Scaling assumptions

Although Grioli restricts his attention to materials with a hyperelastic response, such a constitutive specification is irrelevant to purposes like his. It suffices to assume, as he did, that the stress measures of Piola type scale as follows:

$$\boldsymbol{F}\tilde{\boldsymbol{T}} = (\boldsymbol{F}\tilde{\boldsymbol{T}})_0 + h(\boldsymbol{F}\tilde{\boldsymbol{T}})_1 + o(h), \quad \boldsymbol{F}\tilde{P} = h(\boldsymbol{F}\tilde{P})_1 + o(h). \tag{4}$$

It is also convenient to record here the postulated dependence of external distance and contact loads on the scale parameter h:

$$\boldsymbol{d}_f = (\boldsymbol{d}_f)_0 + h(\boldsymbol{d}_f)_1 + o(h), \quad etc.. \tag{5}$$

2.4. Hierarchy of field and boundary equations

A hierarchical h-sequence of field and boundary equations ensues from a formal combination of the balance laws (1)–(2) with the scaling assumptions (4)–(5) about external loads, namely,

$$\left.\begin{array}{c} \mathrm{Div}(\boldsymbol{F}\tilde{\boldsymbol{T}})_0 + (\boldsymbol{d}_f)_0 = \boldsymbol{0} \quad \text{in } C, \\ \mathbb{e}[(\boldsymbol{F}\tilde{\boldsymbol{T}})_0\boldsymbol{F}^T] + (\boldsymbol{d}_c)_0 = \boldsymbol{0} \quad \text{in } C, \\ (\boldsymbol{F}\tilde{\boldsymbol{T}})_0\boldsymbol{n} = (\boldsymbol{c}_f)_0 \quad \text{and} \quad \boldsymbol{0} = (\boldsymbol{c}_c)_0 \quad \text{in } \partial C; \end{array}\right\} \tag{6}$$

$$\left.\begin{array}{c} \mathrm{Div}(\boldsymbol{F}\tilde{\boldsymbol{T}})_1 + (\boldsymbol{d}_f)_1 = \boldsymbol{0} \quad \text{in } C, \\ \mathrm{Div}(\boldsymbol{F}\tilde{P})_1 + \mathbb{e}[(\boldsymbol{F}\tilde{\boldsymbol{T}})_1\boldsymbol{F}^T] + (\boldsymbol{d}_c)_1 = \boldsymbol{0} \quad \text{in } C, \\ (\boldsymbol{F}\tilde{\boldsymbol{T}})_1\boldsymbol{n} = (\boldsymbol{c}_f)_1 \quad \text{and} \quad (\boldsymbol{F}\tilde{P})_1\boldsymbol{n} = (\boldsymbol{c}_c)_1 \quad \text{in } \partial C; \end{array}\right\} \tag{7}$$

etc..

As to the zero-order system (6), note that it comes to coincide with the Cauchy system of field and boundary equations – that is, with system (4.34)–(4.35) of [2] – whenever the zero-order couple loads $(\boldsymbol{d}_c)_0$ and $(\boldsymbol{c}_c)_0$ are both null; in particular, condition $(\boldsymbol{d}_c)_0 \equiv \boldsymbol{0}$ is satisfied if and only if the Cosserat stress field $(\tilde{\boldsymbol{T}})_0$ is symmetric-valued. Both in [2] and in [1], Grioli questions the general 'physical concreteness' of non-null couple loads of order zero; in [2], he mentions the example of magnetic dipoles in a magnetic field to argue that generally $\lim_{h\to 0} \boldsymbol{d}_c$ should be null; and he reasons that a body can only match null zero-order contact couples at its boundary, because $(4)_2$ implies that $\lim_{h\to 0}(\boldsymbol{F}\tilde{P})\boldsymbol{n} = \boldsymbol{0}$.

Under the assumption that $(\boldsymbol{c}_c)_0 \equiv \boldsymbol{0}$, Grioli regards system (6)–(7) as a first 'refinement of the classic theory of Cauchy', a refinement where only the zero-order stress $(\tilde{\boldsymbol{T}})_0$ (possibly asymmetric in case $(\boldsymbol{d}_c)_0 \neq \boldsymbol{0}$) is physically significant, whereas $(\tilde{\boldsymbol{T}})_1$ and $(\tilde{P})_1$ (as well as all higher-order stress-like constructs) need not be given any 'physical meaning' [1].

2.5. *On the model's physical concreteness*

Irrespectively of the value of the scale parameter h, let the contact fields

$$\hat{\boldsymbol{c}}_f(X,\boldsymbol{n}) := (\boldsymbol{F}\tilde{\boldsymbol{T}})(X)\boldsymbol{n}, \quad \hat{\boldsymbol{c}}_c(X,\boldsymbol{n}) := (\boldsymbol{F}\tilde{P})(X)\boldsymbol{n} \tag{8}$$

be defined at each point $X \in C$ for $\boldsymbol{n}$ the normal to each oriented plane through that point. Then, as is the case for Cauchy continua, it would be possible to induce from relations (8) that *the information content of the stress field* $\boldsymbol{F}\tilde{\boldsymbol{T}}(X)$ $[\boldsymbol{F}\tilde{P}(X)]$ *is the same as that of the contact field* $\hat{\boldsymbol{c}}_f(X,\cdot)$ $[\hat{\boldsymbol{c}}_c(X,\cdot)]$; granted this, at each point $X \in \partial C$ and for $\boldsymbol{n}(X)$ the normal to ∂C at that point, the boundary conditions (2) would read:

$$\hat{\boldsymbol{c}}_f(X,\boldsymbol{n}(X)) = \boldsymbol{c}_f(X), \quad \hat{\boldsymbol{c}}_c(X,\boldsymbol{n}(X)) = \boldsymbol{c}_c(X). \tag{9}$$

Thus, within the mathematical model considered by Grioli in [1, 2], *the 'physical concreteness'* ([1], p. 446) *of the stress fields* $\boldsymbol{F}\tilde{\boldsymbol{T}}$ *and* $\boldsymbol{F}\tilde{P}$ *is the same as that of the contact actions realizable at boundary points and of the contact interactions detectable at interior points.*

3. Continuum theories intended to bridge the micro→macro gap

What in [1] Grioli calls the Cauchy theory, aka the theory of *simple continua*, is a one-velocity and one-gradient field theory, that is to say, a theory where the first partial derivatives with respect to time and space of the only unknown, a time-dependent deformation field over a space region, suffice for a *macroscopic* description of the mechanical vicissitudes of that region.

All theories of *non-simple* (aka *complex*) *continua* are either *multivelocity* or *multigradient*, or both [3]; all attempt to bridge, somehow and to some judicious extent, the micro→macro gap. For example, Grioli's hierarchical theory of microstructures considered in the previous section is multivelocity, while the theories of second-gradient materials considered in [4, 5] contemplate only one velocity field; and, provided temperature is regarded as the time rate of the thermal displacement [6, 7], thermomechanics is indeed a multivelocity theory, with temperature the additional velocity-like variable.

Multigradient theories are meant to account for *nonlocality* in the material response, a challenge that the community studying fractional mechanics has taken up in a systematical manner. Intrinsically nonlocal theories have been considered since long by Edelen [8] and Eringen [9] and, more recently, by Silling and others [10]; consideration of such theories falls beyond the scope of this paper.

As to multivelocity theories, whatever the physical interpretations of the 'velocities' listed in addition to the time rate of mechanical displacement, their true nature is *mesoscopic*, in that the role of the additional velocities is to enrich a purely mechanical macroscopic description of a target physical phenomenology by accounting for certain collective characters of the *microscopic* individual motions. In fact, in such continuum mechanical theories some of the state variables are meant to carry gross information about a large collection of 'substates'.

For example, in classical thermoelasticity, temperature has a psychological status different from displacement gradient: the latter measures macroscopic local changes in shape, volume, or orientation, the former is meant to account for infinitely many, grossly equivalent substates of *microscopic agitation*. *Order parameters* have a role not different from that of temperature, in that they also account for certain substate changes that we do envisage as physically relevant and yet we can not, and at times we choose not to describe in greater detail. However, as the modifier 'order' suggests, the relative substate changes are rather in *microscopic organization* than in microscopic agitation: think, for example, of the order parameter in Allen–Cahn's theory of phase segregation.

Be they multivelocity or multigradient, all theories of complex continua may be given a Virtual Power format; Grioli's theory in [1, 2] is no exception. Power expenditures, no matter if effective or virtual, are scalar quantities and hence can be added up *whatever the space scale* at which they occur. The nature of VP statements is *pre-variational*, in that their formulation may be, but need not be, interpreted as an integral form of the Euler-Lagrange stationarity condition associated with the minimization of some energy functional. Just as for the choice of a class of test functions in the calculus of variations of a functional, the crucial step in the formulation of a VP principle is the choice of a class of virtual velocities, a properly invariant and properly inclusive class, consistent with the 'hard' (aka 'Dirichlet') boundary conditions, if any (in [1], virtual velocities are denoted by $(\delta \boldsymbol{u}, \delta \boldsymbol{R})$; for examples of invariance and inclusiveness requirements, see [4, 5]); ultimately, as is well-known, a VP principle consists in the assertion that two linear and continuous functionals over the collection of virtual velocities, one for the internal the other for the external power expenditure, take equal values at the same velocity field. The predictive power of VP statements depends on their *part-wise quantification*: it is maximal when they are assumed to hold *for all space-time parts* of a chosen Cartesian product of a material body and a time interval. In this instance, *a VP approach produces consistent sets of evolution equations and initial/boundary conditions*.

To exemplify the results of this approach, a modicum of technicalities is inevitable. We let $\mathscr{P}$ denote the open and bounded space region with complete boundary $\partial\mathscr{P}$ occupied at some initial time t_{in} by a typical subbody, and we let I denote a typical open time interval, whose boundary ∂I consists of its end points t_{in} and t_{fin}; moreover, we let the boundary of the space-time part $\mathscr{P} \times I$ be the union of the sets $\partial\mathscr{P} \times \mathscr{I}$ and $\mathscr{P} \times \partial\mathscr{I}$; finally, we let $\partial_h\mathscr{P} \times I$ and $\mathscr{P} \times \{t_{fin}\}$ the 'hard' parts of the boundary of $\mathscr{P} \times I$, where virtual velocity fields must be taken identically null. With this, exploitation of a VP approach simultaneously produces *evolution equations* holding in $\mathscr{P} \times I$, as many as the gradients of the independent velocity-like variables needed to characterise the deformational vicissitudes of the material body under study; *'soft' boundary conditions* holding on $\partial_s\mathscr{P} \times I$ $(\partial_s\mathscr{P} = \partial\mathscr{P} \backslash \partial_h\mathscr{P})$; and *velocity initial conditions* holding on $\mathscr{P} \times \{t_{in}\}$. I reckon that such evolution equations, boundary conditions, and initial conditions, in that they all follow from one and the same mathematical statement, have one and the same collective physical concreteness in the sense of Grioli [1].

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