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MICROSTRUCTURES AND GRANULAR MEDIA

Abstract. A general model of solids with vectorial microstructures is introduced. The field equations are obtained as Euler-Lagrange equations of a suitable energetic functional. The Cosserat model is encompassed in this model and it can be used to study the behaviour of granular media. A first approach to this problem deals with a two dimensional model, since in such a case the field equations have a simpler form, the rotation of the single grain depends on one parameter only, the angle of rotation, but the model is still physically meaningful. In order to obtain constitutive equations rigorously deduced from the principles of Continuum Mechanics, we must take in account both the interaction matrix-grains and grain-grain. As a first step, we deal with linear dissipation, as already done in general for vector microstructures, such that we can also study some simpler problems of wave propagation.

Key words : Microstructures, Cosserat solids, granular media.

1. Introduction

A wide class of phenomena can be described by means of microstructural models of solids and fluids, where the microstructure can be described by vector fields over the body. In principle, there are no restrictions on the number of vector fields, which are unknown variables of the problem, but there are obvious restrictions due to the possible physical meaning of each vector field.

The use of the Cosserat continuum theory to describe the behaviour of granular materials or powders has been proposed in several papers (see, for instance, Grekova [7] and references therein quoted). Basically we refer to [14], but we follow a different approach, in the framework of a general theory of microstructures as developed by Capriz [1], Maugin [8]. In particular we deal with a so-called vector microstructure, which includes the Cosserat theory. This theory has already been used with some success by Pastrone and others [2, 3, 4, 10, 11, 12] to study wave propagation in one and three-dimensional microstructured solids.

In Section 2, the three dimensional Cosserat model is introduced. A Cosserat microstructure is defined by a triple vector field $\{\mathbf{d}_i\}$, such that $\mathbf{d}_i \cdot \mathbf{d}_j = \delta_{ij}$. The vector fields $\mathbf{d}_i = \mathbf{d}_i(X^h, t)$ are often called “directors”, where X^h 's are the Lagrangian coordinates of a point \mathbf{X} in a reference configuration of the body which represents the grain, and t is time. The main feature of such a microstructure is its rotation, which is expressed through an angular velocity vector and a “spatial” spin tensor. The basic equations of motion in the three-dimensional case are derived via a variational principle. In fact, we assume the existence of a strain energy function and we take in account the dissipation by means of the expression of the total power expended.

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The case of a plane Cosserat solid is introduced in Section 3, which can be used to model plane granular media. By this way, the model is much more simplified since we restrict our attention to a two-dimensional plane body. The rotation is fully described by a scalar function $\theta = \theta(X^h, t)$ and the field equations reduce to four differential equations. Some interesting identities are derived, such that we can easily compare our model with

that one introduced by [14] in a general context and used by [7], but we do not neglect the coupled-stress. On the other side, we prove that the stress tensor is not symmetric (as natural in such models) and its skew symmetric part is related to the micro body force. Finally, alternative forms of the field equations are provided.

In Section 4, we make a first step toward the introduction of appropriate constitutive equations, taking into account the friction among particles and describing this phenomenological aspect through a dissipation function whose explicit form is suggested by the total power expended in any motion. A simple example, obtained after further simplifications on the dissipation function, is provided, but the problem of a correct constitutive theory for such models is not solved and it will be the main subject of further researches.

2. Vectorial microstructures

The usual approach to microstructure is assumed to be that one introduced by Mindlin [9], where the model is the linear theory of elasticity. We follow his basic ideas for the kinematics, but in the general framework of non linear elasticity, both in the macro and in the micro-structure. We will obtain a model which could be, somehow, encompassed in the model of Capriz, even though it is not a straightforward procedure.

Let \mathcal{B} be the body, as a manifold embedded in a 3-dimensional affine space, \mathbf{X} a point of this body in its reference configuration C^* , and \mathbf{x} the corresponding point in the actual configuration C . As usual, the displacement is given by the vector function

$$(2.1) \quad \mathbf{u} \equiv \mathbf{x} - \mathbf{X}$$

and, assuming the coordinates X^h of \mathbf{X} as material coordinates, for any motion it will be: $\mathbf{u} = \mathbf{u}(X^h, t)$, since $\mathbf{x} = f(\mathbf{X}, t)$, where f is the deformation function ($f : C^* \rightarrow C$).

The macrostructure is a three-dimensional body \mathcal{B} , and it can be equivalently be described by a position vector, from some fixed origin \mathbf{o} , $\mathbf{r} \equiv \mathbf{x} - \mathbf{o}$, $\mathbf{r} = \mathbf{r}(X^h, t)$ where the X^h 's are material coordinates and t is time. Commas denote partial derivatives with respect to X^h and superposed dots denote partial derivatives with respect to time, e.g.:

$$\mathbf{r}_{,h} \equiv \frac{\partial \mathbf{r}}{\partial X^h}, \quad \dot{\mathbf{r}} \equiv \frac{\partial \mathbf{r}}{\partial t}$$

By microstructure we mean that it is possible to apply a microscope to each point $\mathbf{x} \in C$ and discover a "small world". As shown elsewhere ([10]), some features of this "small world" can be captured by a suitable set of vectors $\mathbf{d}_H = \mathbf{d}_H(\mathbf{X}, t)$,

$H = 1, 2, \dots, n$, which can be called "directors" and represent the micromotion. Their number depends on the physical aspects we want to describe. In the present case, we can reduce this number to three or less, hence we shall use the same lower case indices as for coordinates: $\mathbf{d}_i = \mathbf{d}_i(\mathbf{X}, t)$, $i = 1, 2, 3$.

The kinetic energy density of the body is defined as a quadratic form in the velocities $\dot{\mathbf{r}}$ and $\dot{\mathbf{d}}_i$:

$$(2.2) \quad T = \frac{1}{2}[\rho(X^h)\dot{\mathbf{r}} \cdot \dot{\mathbf{r}} + 2\rho^i(X^h)\dot{\mathbf{r}} \cdot \dot{\mathbf{d}}_i + \rho^{ij}\dot{\mathbf{d}}_i \cdot \dot{\mathbf{d}}_j].$$

In Eq. (2.2), ρ is the usual three dimensional mass density, ρ^i and ρ^{ij} are coefficients including density and inertia terms, which must satisfy the conditions:

$$T \geq 0, \quad T = 0 \Leftrightarrow \dot{\mathbf{r}} = \dot{\mathbf{d}}_i \equiv 0.$$

As it is well-known, it is always possible to diagonalize the form making linear transformations on \mathbf{r} and \mathbf{d}_i , such that

$$\rho^i = 0, \rho^{ij} = \rho I^{ij};$$

the I^{ij} 's are effective inertia terms of the microstructure.

We assign a strain energy density function

$$(2.3) \quad \hat{W} = W(\mathbf{r},_i; \mathbf{d}_j; \mathbf{d}_{j,h}; X^h) + W_b$$

whose existence follows from the assumption that the total power expended P_T is given by $P_{\hat{W}} = d\hat{W}/dt$ and the total energy is given by

$$(2.4) \quad E = \int_B (T - W)\rho \, dX^1 dX^2 dX^3 - \int_B W_b \rho \, dX^1 dX^2 dX^3$$

where W_b is the potential of the external body forces, which depends on \mathbf{r} and X^h only. We avoid internal constraints and leave apart the problem of the boundary conditions.

The equations of motion can be derived as the Euler-Lagrange equations of the energy functional $\varepsilon = \int_{t_0}^{t_1} E dt$:

$$(2.5) \quad \left\{ \begin{array}{l} \left(\frac{\partial W}{\partial \mathbf{r},_i} \right)_{,i} - \frac{\partial W_b}{\partial \mathbf{r}} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{r}}} \\ \left(\frac{\partial W}{\partial \mathbf{d}_{j,i}} \right)_{,i} - \frac{\partial W}{\partial \mathbf{d}_j} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{d}}_j} \end{array} \right.$$

Since the microstructure can have a dissipative effect, we introduce dissipation in the field equations Eqs. (2.5). The deformation velocities are given by

$$(2.6) \quad \dot{\mathbf{r}} = \frac{\partial \mathbf{r}}{\partial t}, \quad \dot{\mathbf{r}},_i = \frac{\partial \mathbf{r},_i}{\partial t}, \quad \dot{\mathbf{d}}_i = \frac{\partial \mathbf{d}_i}{\partial t}, \quad \dot{\mathbf{d}}_{i,j} = \frac{\partial \mathbf{d}_{i,j}}{\partial t}.$$

The total power expended is the sum of scalar products as it follows:

$$(2.7) \quad P_T = \mathbf{b} \cdot \dot{\mathbf{r}} + \sum_i \boldsymbol{\sigma}_i \cdot \dot{\mathbf{r}}_{,i} + \sum_i \boldsymbol{\tau}_i \cdot \dot{\mathbf{d}}_i + \sum_{ij} \boldsymbol{\eta}_{ij} \cdot \dot{\mathbf{d}}_{i,j},$$

The quantities \mathbf{b} , $\boldsymbol{\sigma}_i$, $\boldsymbol{\tau}_i$, $\boldsymbol{\eta}_{ij}$ are forces, stresses and generalized (or coupled) stresses.

We can split the “conservative” part from the dissipation by means of the decomposition:

$$(2.8) \quad P_T = P_{\hat{W}} + P_D = \frac{d\hat{W}}{dt} + P_D$$

where $P_D = \hat{\mathbf{b}} \cdot \dot{\mathbf{r}} + \sum_i \hat{\boldsymbol{\sigma}}_i \cdot \dot{\mathbf{r}}_{,i} + \sum_i \hat{\boldsymbol{\tau}}_i \cdot \dot{\mathbf{d}}_i + \sum_i \hat{\boldsymbol{\eta}}_{ij} \cdot \dot{\mathbf{d}}_{i,j}$, the hat meaning that we deal with the dissipative part of the stresses, or the so-called non-equilibrium stresses. The dissipation implies $P_D > 0$ for any admissible deformation, hence the non-equilibrium stresses cannot be arbitrary, but they must satisfy this inequality.

Finally the stresses can be written in the additive form

$$(2.9) \quad \left\{ \begin{array}{l} \mathbf{b} = -\frac{\partial W_b}{\partial \mathbf{r}} + \hat{\mathbf{b}} \\ \boldsymbol{\sigma}_i = \frac{\partial W}{\partial \mathbf{r}_{,i}} + \hat{\boldsymbol{\sigma}}_i \\ \boldsymbol{\tau}_i = -\frac{\partial W}{\partial \mathbf{d}_i} + \hat{\boldsymbol{\tau}}_i \\ \boldsymbol{\eta}_{ij} = \frac{\partial W}{\partial \mathbf{d}_{i,j}} + \hat{\boldsymbol{\eta}}_{ij} \end{array} \right.$$

and the field equations read

$$(2.10) \quad \left\{ \begin{array}{l} \boldsymbol{\sigma}_{i,i} + \mathbf{b} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{r}}} \\ \boldsymbol{\eta}_{ij,j} + \boldsymbol{\tau}_i = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{d}}_i} \end{array} \right.$$

which obviously include (2.5). In many cases the body forces are neglected, hence $\mathbf{b} = \mathbf{0}$ and the microbody force included in $\boldsymbol{\tau}_i$ vanishes as well, but $\boldsymbol{\tau}_i \neq 0$, because the coupling part remains.

3. 3-D Cosserat solids

Let us introduce Cosserat solids as a particular model of vectorial microstructure and obviously it can encompass Cosserat shells and rods as well. In Cosserat models the microstructure is described by a rigid triad $\{\mathbf{d}_i\}$, which is attached to each particle of the body. It means that one must add to our field equations (2.5) the constraint equations:

$$(3.1) \quad \mathbf{d}_i \cdot \mathbf{d}_j = \delta_{ij}.$$

Formally we can apply the Lagrange multipliers method to the energy functional

$$(3.2) \quad \mathcal{E} = \int_{\mathcal{B}} [W + \Lambda^{ij} (\mathbf{d}_i \cdot \mathbf{d}_j - \delta_{ij}) + T] d\mathcal{B}$$

and easily derive the equations of motion as a determined set of partial differential equations

$$(3.3) \quad \begin{cases} \left(\frac{\partial W}{\partial \mathbf{r}_i} \right)_{,i} - \frac{\partial W_b}{\partial \mathbf{r}} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{r}}} \\ \left(\frac{\partial W}{\partial \mathbf{d}_j} \right)_{,i} - \frac{\partial W}{\partial \mathbf{d}_j} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{d}}_j} - 2\Lambda^{ij} \mathbf{d}_i \\ \mathbf{d}_i \cdot \mathbf{d}_j = \delta_{ij} \end{cases}$$

Moreover they contain the constraint reactions (namely, the Lagrange multipliers) while the main interest here is to obtain equations of motion free of reactions, sufficient to determine the motion.

This goal can be attained following an intrinsic approach, by means of the angular velocity $\boldsymbol{\omega}$ such that

$$(3.4) \quad \dot{\mathbf{d}}_i = \boldsymbol{\omega} \times \mathbf{d}_i$$

(since we deal with a rigid microstructure), with

$$(3.5) \quad \boldsymbol{\omega} = \boldsymbol{\omega}(q^i, \dot{q}^i, t), \quad q^i = q^i(X^h, t)$$

being suitable measures of the rotations in an affine three-dimensional E_3 (i.e., Euler angles), and a “spatial spin” $\Omega \in Lin$ such that

$$(3.6) \quad \mathbf{d}_{i,h} = \varepsilon_{ij}^k \Omega_h^j \mathbf{d}_k$$

where ε_{ij}^h is the Levi-Civita symbol, and $\Omega = \Omega(q^i, q^i, h, t)$. Henceforth, we can write

$$(3.7) \quad \begin{cases} W = W(\mathbf{r}_i, \Omega, x^h) \\ T = T(\dot{\mathbf{r}}, \boldsymbol{\omega}) \end{cases}$$

where T is a quadratic form in the variables $\dot{\mathbf{r}}$ and \dot{q}^i .

At this point we have to apply the usual variational techniques to the functional

$$(3.8) \quad \mathcal{E} = \int_{\mathcal{B}} [W(\mathbf{r}_i, \Omega, X^h) + T(\dot{\mathbf{r}}, \boldsymbol{\omega})] d\mathcal{B}.$$

The Lagrange equations are (3.3)₁ and

$$(3.9) \quad \partial_i W - \partial_h \partial_i^h W + \partial_i T - \frac{d}{dt} \frac{\partial T}{\partial \dot{q}^i} = 0$$

where

$$\partial_i W = \frac{\partial W}{\partial \Omega} \frac{\partial \Omega}{\partial q^i}, \quad \partial_i T = \frac{\partial T}{\partial \omega} \frac{\partial \omega}{\partial q^i}, \quad \partial_h \partial_i^h W = \frac{\partial}{\partial X^h} \frac{\partial W}{\partial q_{,h}^i} = \frac{\partial}{\partial X^h} \frac{\partial W}{\partial \Omega} \frac{\partial \Omega}{\partial q_{,h}^i}.$$

If we introduce

$$W_\Omega \equiv \frac{\partial W}{\partial \Omega}, \quad T_\omega \equiv \frac{\partial T}{\partial \omega}$$

the equations of Cosserat microstructure can be written as

$$(3.10) \quad \begin{cases} \left(\frac{\partial W}{\partial \mathbf{r}_{,i}} \right)_{,i} - \frac{\partial W_b}{\partial \mathbf{r}} & = \frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{r}}} \\ \left(W_\Omega \frac{\partial \Omega}{\partial q_{,h}^i} \right)_{,h} - W_\Omega \frac{\partial \Omega}{\partial q^i} & = \frac{d}{dt} \left(T_\omega \frac{\partial \omega}{\partial \dot{q}^i} \right) - T_\omega \frac{\partial \omega}{\partial q^i} \end{cases}$$

An open problem is to write the (known) explicit expression of ω in terms of the q^i and \dot{q}^i and the explicit expressions of the spin in terms of the $q^i, q_{,h}^i$, hence to write down explicit forms of the strain energy functions, such that the field equations become suitable and useful both to obtain analytical results and for applications.

4. 2-D Cosserat solids and plane granular media

If the body is a 2-D solid and its configuration at any time is a domain contained in \mathbb{R}^2 , we can choose an orthonormal spatial basis $\{\mathbf{e}_h\}$, $h = 1, 2$ and a material basis $\{\mathbf{g}_h\}$, where $\mathbf{g}_h = \mathbf{r}_{,h}$, hence write $\mathbf{r} = x^h(X^k, t)\mathbf{e}_h$; the functions $x^h(X^k, t)$ have the meaning of deformation function components.

The director fields can be reduced to one vector field $\mathbf{d} = \mathbf{d}(X^k, t)$, $\mathbf{d} \cdot \mathbf{d} = 1$, because one director is sufficient to define the orientation of any particle (grain). In the spatial basis it is: $\mathbf{d} = \cos \theta \mathbf{e}_1 + \sin \theta \mathbf{e}_2$, $\theta = \theta(X^k, t)$ being the angle of rotation of the particle with respect to the fixed basis. Physically, we interpret \mathbf{d} as the kinematical characterization of the grain and it is fully determined by the scalar function $\theta(X^k, t)$. If we introduce the unit vector $\mathbf{v} = -\sin \theta \mathbf{e}_1 + \cos \theta \mathbf{e}_2$, $\mathbf{v} \cdot \mathbf{d} = 1$, the time and spatial derivatives of the director are given by:

$$\dot{\mathbf{d}} = \boldsymbol{\omega} \times \mathbf{d} = \dot{\theta} \mathbf{v}, \quad \mathbf{d}_{,h} = \boldsymbol{\Omega}_h \times \mathbf{d} = \theta_{,h} \mathbf{v},$$

where $\boldsymbol{\omega} = 1/2 \dot{\mathbf{d}} \times \mathbf{d}$, $\boldsymbol{\Omega}_h = 1/2 \mathbf{d}_{,h} \times \mathbf{d}$. The kinetic energy density becomes

$$(4.1) \quad T = \frac{1}{2} [\rho \dot{\mathbf{r}} \cdot \dot{\mathbf{r}} + 2J \dot{\mathbf{r}} \cdot \dot{\mathbf{d}} + I \dot{\theta}^2]$$

where $\rho = \rho(X^h)$ is the density in a reference configuration, $I = I(X^h)$ the inertia term of the grain, J a coupled inertia term that vanishes if we reduce T to a diagonal form, as always possible. The strain energy density becomes

$$(4.2) \quad W = W(x^h_{,k}; \theta; \theta_{,k}; t)$$

while it is convenient to split the potential of the body forces in two parts

$$(4.3) \quad W_b = W_b^{Macro}(x^h, t) + W_b^{micro}(\theta, t)$$

such that the total potential energy density is given by

$$(4.4) \quad \hat{W} = W + W_b^{Macro} + W_b^{micro},$$

the total energy of the body by

$$(4.5) \quad E = \int_A (T - \hat{W})\rho dX^1 dX^2$$

where A is the domain in \mathbb{R}^2 occupied by the reference configuration.

The field equations now read

$$(4.6) \quad \begin{cases} \left(\frac{\partial W}{\partial x^{h,i}} \right)_{,i} - \frac{\partial W_b^{Macro}}{\partial x^h} = \frac{d}{dt} \frac{\partial T}{\partial \dot{x}^h} = \rho \ddot{x}^h \\ \left(\frac{\partial W}{\partial \theta,i} \right)_{,i} - \frac{\partial W}{\partial \theta} - \frac{\partial W_b^{micro}}{\partial \theta} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\theta}} = I \ddot{\theta} \end{cases}$$

In Eq. (4.6) we used the diagonal form for the kinetic energy

$$(4.7) \quad T = \frac{1}{2}[\rho \delta_{ij} \dot{x}^i \dot{x}^j + I \dot{\theta}^2]$$

The power expended for any motion

$$(4.8) \quad P = \frac{\partial \hat{W}}{\partial x^h} \dot{x}^h + \frac{\partial \hat{W}}{\partial x^{h,k}} \dot{x}^{h,k} + \frac{\partial \hat{W}}{\partial \theta} \dot{\theta} + \frac{\partial \hat{W}}{\partial \theta,h} \dot{\theta}_{,h}$$

suggests us how to introduce the macro and micro stresses

$$(4.9) \quad \sigma_k^h = \frac{\partial \hat{W}}{\partial x^{k,h}}, \quad \eta^h = \frac{\partial \hat{W}}{\partial \theta,h}, \quad \tau = \frac{\partial \hat{W}}{\partial \theta}$$

and the macro and micro body forces

$$(4.10) \quad B_h = \rho \frac{\partial W_b^{Macro}}{\partial x^h}, \quad b = \rho \frac{\partial W_b^{micro}}{\partial \theta}$$

which we refer to intrinsically as $\{\sigma, \eta, \tau, \mathbf{B}, b\}$. Hence the field equations read

$$(4.11) \quad \begin{cases} \rho \ddot{\mathbf{u}} = \text{Div} \sigma + \rho \mathbf{B} \\ I \ddot{\theta} = \text{Div} \eta - \tau + \rho b \end{cases}$$

5. The constitutive equations

The system in Eq. (4.6), or alternatively Eqs. (4.11), must be completed with proper constitutive equations, which allow us to describe the behaviour of some real material. If we want to model the behaviour of granular media, we must take into account the friction among grains, which are described kinematically and dynamically as Cosserat microstructures. One way to describe this kind of friction is to make use of the theory of viscosity or, equally, to introduce some dissipation, that means we assume a dependence of the constitutive functions on the velocity of deformation also. Moreover, from a phenomenological point of view we must consider that the rotation of a single grain makes the other neighbouring grains to rotate, not in the same sense: usually, because of friction, if a grain rotates clockwise, another grain in contact with it rotates counter-clockwise. This problem has been faced by [7], using a different approach.

The form of the total power expended, where we must take into account both the conservative and dissipative parts of the stresses, can suggest the choice of the dissipation function. Hence, we assume again that the stresses are “split” in an additive way, so we can write:

$$(5.1) \quad P_T = P_{\hat{W}} + P_D = \frac{d\hat{W}}{dt} + \sigma_D \cdot L + \eta_D \cdot \dot{\mathbf{G}} + \tau_D \dot{\theta}$$

where L is the gradient of the macro velocity, $\dot{\mathbf{G}}$ the gradient of the micro velocity. In Eq. (5.1) σ_D , η_D , τ_D are the dissipative parts of stress and forces (or, as said above, the non-equilibrium stresses and forces). They must satisfy the dissipation inequality

$$(5.2) \quad P_D = \sigma_D \cdot L + \eta_D \cdot \dot{\mathbf{G}} + \tau_D \dot{\theta} > 0$$

for any admissible motion.

The simplest meaningful assumption we can use on the dissipation is that $\sigma_D \cdot L + \eta_D \cdot \dot{\mathbf{G}} = 0$ and $\tau_D = D$, such that $P_D = D\dot{\theta}$ and $D = D(X^i, t)$.

Finally, the simpler form of the field equations for a granular plane body, with friction among grains, is given by

$$(5.3) \quad \begin{cases} \rho \ddot{x}^h = \left(\frac{\partial W}{\partial x^{h,i}} \right)_{,i} + \rho B^h \\ I \ddot{\theta} = \left(\frac{\partial W}{\partial \theta_{,i}} \right)_{,i} - \frac{\partial W}{\partial \theta} - D\dot{\theta} + \rho b \end{cases}$$

Obviously, one can imagine more complicated situations, for instance that the dissipation is given by non linear relations or by a functional in the velocities of deformation, but this model, extremely simple, allows us to claim that it is not necessary to neglect the couple stress, as assumed in [7].

The different equations of motions here obtained allow us to study problems of equilibrium, stability, wave propagation. With regard to wave propagation, some

results have been obtained in [2, 3, 4, 5, 10, 11, 12, 13], mainly in one-dimensional solids with scalar microstructure, with non linearity, dispersion and dissipation. The possibility of propagation of solitary waves has been proved, as well as the possibility of decay and/or amplification of the amplitude.

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