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Extended continuum mechanics for the study of granular flows

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Fisica matematica. — *Extended continuum mechanics for the study of granular flows.*
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ABSTRACT. — We exploit a recent proposal of an «extended kinematics» to describe fast flows of granular materials. Prompted by some remarks in elementary point dynamics, we suggest balance laws which might be of use in studying the evolution of those flows.

KEY WORDS: Granular materials; Fast flow; Extended mechanics.

RIASSUNTO. — *Meccanica dei continui «estesa» per lo studio di flussi granulari.* Una recente proposta per una «cinematica estesa» è sfruttata per la descrizione di flussi rapidi in continui granulari. Sulla base di alcuni corollari della dinamica elementare, si suggeriscono equazioni di bilancio che possono servire nello studio di tali flussi.

1. INTRODUCTION

A mathematical description of the fast flow of a granular material cannot be achieved merely by an appropriate choice of the constitutive function for the stress, as though the material were an ordinary continuum obeying only the classical balance laws of mass, momentum, moment of momentum. The fluctuations of velocity in the neighbourhood of any point are usually large and moreover the «particles» involved are not as minute as happens in gases. Also, the link between gross motion and local agitation seems to be more direct than in gases, so that a nominal split of gross mechanical phenomena from underlying «thermal» discord has less ground. Nevertheless one may profit from ideas emerging in the kinetic theory of gases as shown in papers by Jenkins *et al.* (see, *e.g.*, [1, 2]).

We follow here another path and move from a remark in [3] which, indeed, suggests an extension of classical continuum mechanics, so as to account for fluctuations of the velocity field in the neighbourhood of any place x . The fluctuations are described by a kinematic tensor $A(x)$, such that, in particular,

$$\alpha = -n \cdot An$$

assigns the self-penetration flow rate through the plane with normal n within the material element centred at x , whereas

$$An + \alpha n = (n \times An) \times n$$

measures the slip rate of one half-element with respect to the other (the splitting of the element in halves being realized by the same plane).

A measure of the intensity of fluctuations could be the quantity $\theta = (1/6)A \cdot A$ (where the factor $1/6$ is introduced for later convenience), a positive number called «granular temperature» in view of many similarities: for instance, θ satisfies

(*) Nella seduta del 13 maggio 1995.

an equation which, as we shall see, coincides formally with the classical heat equation.

By use of the tensor A , or, at least, of the associated symmetric tensor

$$(1.1) \quad H = \frac{1}{3} AA^T,$$

details of the flow may be evidenced, which would escape the usual macroscopic analysis. To determine A , another dynamic equation must be added to the classical ones, thus engendering an «extended» continuum mechanics; actually, the adjective «extended» is borrowed from papers on thermodynamics by Ingo Müller *et al.* (see, e.g., [4]). Our debit to those papers is deeper than terminological; we come here to an extended set of balance equations, as they do, and as happens in Grad's 13-moment theory.

2. EXTENDED KINEMATICS

In this section we first recall briefly the relevant remark from [3], which suggests a way of accounting, within a slightly enlarged classical continuum scheme and at least roughly, for the discordant motion of agitation of the molecules (or granules) around a place x . It is suggested there:

(i) to consider, at each place x and time t , together with the usual «spherical» mass-weighted mean $v(x, t)$ of the molecular (or granular) velocities, also the «hemispherical» means obtained from the two subsets, of the spherical neighbourhood, bounded by the plane of unit normal vector n ;

(ii) to take their difference $w(x, t; n)$, odd in n , and to assume valid a linear estimate

$$(2.1) \quad w(x, t; n) = A(x, t)n,$$

where A is an appropriate second order tensor, which will be used to portray the agitation of the granules.

Having in mind later applications, we introduce specific jargon: the material element of [1] will be called here a «chunk» of material. It is a sort of quasi-particle; it should contain a fair number of granules (or pebbles), otherwise the estimate (2.1) could only be very poor. Assume, outrageously but for the sake of argument, that the chunk contain only two granules of equal mass with opposite fluctuation speed s and $-s$ respectively. Then w would be equal to $2s$ for all n such that the corresponding half-space contain the granule with speed s ; and $-2s$ in the contrary instance, with a jump through 0. An «approximation» allowed by (2.1) could be

$$A = \frac{\sqrt{3}s \otimes s}{|s|},$$

the factor $\sqrt{3}$ here being required to conserve the «temperature» (see (2.2) below).

The tensor A need not be symmetric; special properties of A apply within special classes of agitations. Trivially, if all granules participate in exactly the same local motion

as described by the local value of the macroscopic velocity v , then all hemispherical means are also equal to v and A is null.

Non-null values of A correspond to non-trivial agitation, with granule speeds distinct from the mean value. For instance, if A is non-null but spherical then one may imagine a more or less violent, purely radial, pulsation within the chunk, as is thought to occur in continua with small and thinly spread spherical voids. If A is skew, then, as is easily ascertained, the agitation could be a rigid rotation with a speed related to the vector z associated with A . Finally, if A is symmetric, then the agitation could have the same properties which are secured by a symmetric value of $\text{grad } v$ in the local specification of the macromotion. The conditional is used above because the mentioned properties of A could apply even for more complex agitations; furthermore, the field of agitation velocities need not be linear in n , as broached in our approximation.

There are a number of interesting quantities associated with A ; perhaps the most important is the «granular temperature» θ , which is in relation with the kinetic energy of agitation per unit mass averaged over all directions n

$$(2.2) \quad \theta := \frac{1}{2(\text{area } S)} \int_S w^2 dS,$$

here S is the unit sphere. One finds

$$(2.3) \quad \theta = \frac{1}{8\pi} (AA^T) \cdot \int_S n \otimes n dS = \frac{1}{6} A \cdot A,$$

because

$$(2.4) \quad \int_S n \otimes n dS = \frac{4}{3} \pi I; \quad (I, \text{ identity tensor}).$$

This result is of the essence, as evidenced later, when we compare properties of the continuum scheme with properties which apply for discrete systems.

2θ is the trace of the tensor H which measures the momentum flux per unit mass:

$$(2.5) \quad H := \frac{1}{\text{area } S} \int_S w \otimes w dS = \frac{1}{\text{area } S} A \left(\int_S n \otimes n dS \right) A^T = \frac{1}{3} AA^T.$$

H could be named also (average) Reynold's tensor, as in fluid dynamics, or kinetic energy operator. The distinct, and prevalent, rôle of H in balance equations suggests the recourse for A to the product decomposition theorem, which asserts the existence of an orthogonal tensor R such that

$$(2.6) \quad A = \sqrt{3} H^{1/2} R.$$

We could call R the «sling» associated with A : in fact, a glance at (2.1) shows that R effects the same rotation on all normals n , giving to our picture of local agitation the essential aspects of a more or less pronounced vortex. The value of R does not influence the instantaneous value of momentum flux, nor, evidently, that of the granular temperature, but may be decisive in determining the energy loss rate due to friction, at

least in some granular flows. The relationship between R and the vector z involves H

$$(2.7) \quad z = \frac{\sqrt{3}}{2} \mathbf{e} H^{1/2} R,$$

here \mathbf{e} is Ricci's permutation tensor.

The agitation's inertia can be expressed, as we shall see, through the time derivative of A , or those of H and R . One finds that

$$(2.8) \quad \dot{A}A^T = 3[(H^{1/2})' H^{1/2} + H^{1/2} \dot{R}R^T H^{1/2}]$$

or, equivalently,

$$(2.9) \quad \begin{cases} 2 \operatorname{sym} \dot{A}A^T = 3 \dot{H}, \\ \operatorname{skw} \dot{A}A^T = 3 \{ \operatorname{skw} [(H^{1/2})' H^{1/2}] + H^{1/2} \dot{R}R^T H^{1/2} \}. \end{cases}$$

Here use is made of the identities

$$\begin{aligned} \dot{Y} &= (Y^{1/2})' Y^{1/2} + Y^{1/2} (Y^{1/2})', & (Y^{-1})' &= -Y^{-1} \dot{Y} Y^{-1}, \\ Y^{1/2} (Y^{-1/2})' &+ (Y^{-1/2})' Y^{1/2} &= -Y^{-1/2} \dot{Y} Y^{-1/2}, \end{aligned}$$

valid for any symmetric, positive definite tensor Y .

3. EXTENDED ELEMENTARY DYNAMICS

Within the continuum model, balance equations for complex materials are usually prompted by equations of motion of elementary mechanics and their corollaries. Even Cauchy's equation can be said to express, for the material element, Newton's axiom; or, rather, when integrated over a region, to express the first Euler equation for the material system occupying that region, in analogy of one derived for a set of mass points. The proposal of the brothers Cosserat is based on ideas from rigid body dynamics; many theories of continua with microstructure are constructed by modelling the material element as a Lagrangian system.

Here, restricting ourselves for the moment to the consideration of an aggregate of mass-points, we derive a corollary of elementary point dynamics, which will prove to be the appropriate tool for our goal, as Euler equations are for the usual purposes. Consider a system \mathcal{C} of points $x^{(i)}$ ($i = 1, 2, \dots, N$) with respective masses $m^{(i)}$, velocities $v^{(i)}$, each acted upon by a force $f^{(i)}$; call m the total mass, v the velocity of the centre of mass and $w^{(i)} = v^{(i)} - v$ the relative velocity of $x^{(i)}$.

Introduce the Reynold's tensor (we use the superscript $\widehat{\langle \rangle}$ to distinguish quantities within the discrete model which are similar to quantities within the continuum model)

$$(3.1) \quad \widehat{H} := \frac{1}{m} \sum m^{(i)} w^{(i)} \otimes w^{(i)},$$

and notice that

$$(3.2) \quad \dot{\widehat{H}} = 2 \operatorname{sym} \widehat{W},$$

if

$$(3.3) \quad \widehat{W} := \frac{1}{m} \sum m^{(i)} w^{(i)} \otimes \dot{w}^{(i)}.$$

Introduce also the vector \widehat{y} associated with the skew part of \widehat{W}

$$(3.4) \quad \widehat{y} = \frac{1}{2} \mathbf{e} \widehat{W}.$$

Then easy developments, starting from Newton's law of point dynamics, lead to the equation of balance

$$(3.5) \quad \frac{1}{2} m \dot{\widehat{H}} + m \mathbf{e} \widehat{y} = \widehat{S},$$

where \widehat{S} is a total which we call the «stir»

$$(3.6) \quad \widehat{S} := \sum w^{(i)} \otimes f^{(i)}.$$

Naturally (3.5) is of good stead only in cases where a sufficiently clear picture of the kinetic behaviour of \mathcal{C} around its centre of mass can be drawn by use of a restricted number of parameters, and, consequently, \widehat{S} can be expressed in terms of (x, v) and those parameters only; for them, hopefully, (3.5) becomes then an evolution equation.

Suppose, for instance, that a tensor \widehat{B} exists, function of time only, such that

$$(3.7) \quad w^{(i)} = \widehat{B}(x^{(i)} - x),$$

as happens trivially when the motion of \mathcal{C} is rigid, \widehat{B} being then skew. Introduce the tensor

$$(3.8) \quad \widehat{J} := \frac{1}{m} \sum m^{(i)} (x^{(i)} - x) \otimes (x^{(i)} - x),$$

which is related with the usual inertia tensor Y thus:

$$\widehat{J} = \frac{1}{2} (\text{tr } Y) I - Y,$$

and remark that

$$(3.9) \quad \dot{\widehat{J}} = \widehat{B}\widehat{J} + \widehat{J}\widehat{B}^T.$$

Again, easy developments lead to the identities

$$(3.10) \quad \widehat{H} = \widehat{B}\widehat{J}\widehat{B}^T, \quad \widehat{W} = \widehat{B}\widehat{J}(\dot{\widehat{B}} + \widehat{B}^2)^T$$

and (3.5) takes the form

$$(3.11) \quad m\widehat{W} = \widehat{S}$$

which is an evolution equation for \widehat{B} , if \widehat{S} is a function of (x, v) and \widehat{B} only.

The predictive character of (3.11) is more immediately evident when \widehat{B} and \widehat{J} are non singular; then one can put (3.11) in normal form

$$(3.12) \quad m(\dot{\widehat{B}} + (\widehat{B}^T)^2) = \widehat{J}^{-1}\widehat{B}^{-1}\widehat{S}.$$

To get near to notation and meanings of sect. 2, one can make use, without substantial change, of the tensor

$$(3.13) \quad \widehat{A} = \sqrt{3} \widehat{B}\widehat{J}^{1/2},$$

instead of \widehat{B} so that the relation (2.5)

$$\widehat{H} = \frac{1}{3} \widehat{A} \widehat{A}^T$$

is formally identical with (1.1).

Also, one may, by use of (3.2), point to an important corollary of (3.12) (or, rather, of (3.5))

$$(3.14) \quad m \dot{\widehat{H}} = 2 \text{sym} \widehat{S}.$$

REMARK 1. The correspondence between quantities introduced in this section and those indicated by the same letters in sect. 2 is not strict; in particular, $(1/2) \text{tr} \widehat{H}$ gives exactly the kinetic energy of the mass-points in their motion relative to the centre of gravity, whereas ϑ in (2.2) gives a lower estimate of the same quantity. It is easy to check that, for the case of the system of mass-points, coincidence would occur if the following equality held

$$y'(n) - y''(n) = \sqrt{3} J^{1/2} n;$$

here y' and y'' are the vectors joining x with the centres of gravity of the two subsystems each within one of the half-spaces bounded by the plane with normal n . In the spirit of continuum theory, we do not worry about such relatively subtle discrepancy and we take (3.13) as the definition of \widehat{A} .

From (2.8), (2.9), (2.10) and the relations

$$(3.15) \quad \left\{ \begin{aligned} \widehat{W} &= \widehat{H}^{1/2} \widehat{R} \widehat{J}^{1/2} (\widehat{J}^{-1/2})' \widehat{R}^T \widehat{H}^{1/2} + \\ &\quad + \widehat{H}^{1/2} \widehat{R} \dot{\widehat{R}}^T \widehat{H}^{1/2} + \widehat{H}^{1/2} (\widehat{H}^{1/2})' + \widehat{H} \widehat{J}^{-1/2} \widehat{R}^T \widehat{H}^{1/2}, \\ \dot{\widehat{J}} &= \widehat{H}^{1/2} \dot{\widehat{R}} \widehat{J}^{1/2} + \widehat{J}^{1/2} \widehat{R}^T \widehat{H}^{1/2}, \end{aligned} \right.$$

one can deduce, finally, the differential equation in R

$$(3.16) \quad m \left\{ \dot{\widehat{R}} \widehat{R}^T + \frac{1}{2} \text{skw} [\widehat{H}^{1/2} \widehat{J}^{-1/2} \widehat{R}^T + (\widehat{H}^{1/2})' \widehat{H}^{-1/2} + \widehat{R} \widehat{J}^{1/2} (\widehat{J}^{-1/2})' \widehat{R}^T] \right\} = \\ = \text{skw} \widehat{H}^{-1/2} \widehat{S} \widehat{H}^{-1/2}.$$

REMARK 2. The consequences of the third axiom of point dynamics are, here, the vanishing of the resultant $\sum f_{\text{int}}^{(i)}$ of all internal forces $f_{\text{int}}^{(i)}$ on \mathcal{C} and of the trace of the stir due to internal actions for any rigid agitation with rotational speed q :

$$(3.17) \quad \sum q \times (x^{(i)} - x) \cdot f_{\text{int}}^{(i)} = q \cdot \sum (x^{(i)} - x) \times f_{\text{int}}^{(i)} = 0,$$

for all q .

4. EXTENDED CONTINUUM MECHANICS

To come to a proposal for a continuum theory inspired by the elementary developments of sect. 3 one must first invoke mass-density ρ , gross velocity v , Cauchy's stress T and the corresponding relevant equations of balance of mass and momentum as in the

classical case; then adjoin further fields W, H, R, S and relate them through additional equations of balance, which must mimic (3.14), (3.16) and (3.17). However, great care must be taken to interpret correctly the significance to be attributed in a continuum scheme to terms appearing in the latter equations, when they are applied to a chunk (and when the mass-points are interpreted as granules perhaps now imagined as spread out continuously within the chunk). One must observe that, though the chunk is not a system with variable mass, some granules may leave \mathcal{C} through $\partial\mathcal{C}$ and others may join, as a result of interactions with other chunks. Secondly, the time derivative of an integral, such as $\int_{\mathcal{C}} \dot{H}$, may be inadequate to represent alone correctly the derivative in the left-hand side of (3.14); one must account separately for the sudden change of momentum in some granules belonging to \mathcal{C} but reflected instantaneously on the boundary $\partial\mathcal{C}$ through collisions due to their agitation with granules not belonging to \mathcal{C} . Both of these additional intrinsic contributions to the rate of change of agitation may be represented by an integral over $\partial\mathcal{C}$, say

$$(4.1) \quad \int_{\partial\mathcal{C}} \mathbf{S}n_e \simeq (\text{vol } \mathcal{C}) \text{div } \mathbf{S},$$

where n_e is the unit vector of the exterior normal to $\partial\mathcal{C}$ and \mathbf{S} is an appropriate third order tensor, the dependence of which on H, R (and quantities related to the gross motion) must be specified by a constitutive law.

REMARK 1. Notice that, in deriving (4.1) and also below, we use «pro tempore» continuum theory at the lower scale inside the chunk. The final relations will be written at the macroscopic scale, but they will contain the essential «residues», as it were, brought «afloat» from our exploration of the lower scale.

Reflections of granules on $\partial\mathcal{C}$ are a consequence not only of factors intrinsic to the chunk, but are generated also by gross velocity gradients. We insinuate the idea that this effect may be accounted for through a component of the stir S . On $\partial\mathcal{C}$ the gross force per unit area is the traction Tn_e , which works against the velocity differential due to the velocity gradient of the gross motion. We suggest that, when the chunk \mathcal{C} is imagined as a sphere \mathcal{S} of radius ε , the value per unit volume be

$$\frac{1}{\text{vol } \mathcal{C}} \int_{\mathcal{S}} [(\text{grad } v) \varepsilon n] \otimes Tn \, dS,$$

or, approximately,

$$\frac{1}{\text{vol } \mathcal{C}} \varepsilon^3 (\text{grad } v) \left(\int_{\mathcal{S}} n \otimes n \, dS \right) T^T,$$

and using (2.4)

$$(4.2) \quad (\text{grad } v) T^T.$$

In conclusion we propose the following version of (3.11) for the continuum scheme

$$(4.3) \quad \rho \dot{W} + \operatorname{div} \mathbf{S} = (\operatorname{grad} v) T^T + S_E + \tilde{S},$$

where S_E is the stir due to actions external to the body such as e.m. actions, \tilde{S} is the contribution to S of internal (dissipative) actions not accounted for by (4.2), and W is defined in terms of A and J as is suggested by (3.10)_{II} and (3.13).

REMARK 2. To accept without qualms the result just obtained one must recall, first of all, the earlier remark in this section. Besides, one must agree on the implicit assumption of a relation between the two scales: so to speak, differentials at the macro scale are taken to be finite quantities at the micro scale. There is a very important additional mechanical implication in the acceptance of (4.2). The quantity (4.2) represents the stir generated by the macromotion; the implication is that it is totally transferred to the motion of agitation without loss in the transfer, or nearly so. Thus the separate term \tilde{S} is deemed sufficient to account for the inelastic losses in collisions. Perhaps, in a more comprehensive theory, such additive decomposition of effects would not always apply.

Immediate corollaries of (4.3) and (3.14), (3.16) are

$$(4.4) \quad \frac{1}{2} \rho \dot{H} = \operatorname{sym} [-\operatorname{div} \mathbf{S} + (\operatorname{grad} v) T^T + S_E + \tilde{S}],$$

$$(4.5) \quad \rho \left\{ \dot{R} R^T + \frac{1}{2} \operatorname{skw} [H^{1/2} J^{-1/2} R^T + (H^{1/2})' H^{-1/2} + R J^{1/2} (J^{-1/2})' R^T] \right\} = \\ = \operatorname{skw} \{ H^{-1/2} [-\operatorname{div} \mathbf{S} + (\operatorname{grad} v) T^T + S_E + \tilde{S}] H^{-1/2} \}.$$

Taking the trace of both members in (4.4) and using (2.3) one obtains also

$$(4.6) \quad \frac{1}{2} \rho \dot{\theta} = -\operatorname{tr} (\operatorname{div} \mathbf{S}) + (\operatorname{grad} v) \cdot T + \operatorname{tr} (S_E + \tilde{S}),$$

which coincides with (30) of [1], when trivial identifications are performed (notice, in particular, that, here, tractions rather than pressures are taken as positive). By subtracting from both members of (4.4) the corresponding member of (4.6) multiplied by $1/3$ of the identity tensor one obtains the balance equation for the deviators, *i.e.* (31) of [1], modulo obvious identifications. Equation (4.4), again with appropriate identifications, coincides also with (3) of [2].

REMARK 3. We have already called θ the granular temperature. If, besides, we interpret the vector q obtained by partial contraction from \mathbf{S} as granular heat flux vector and the scalar $\operatorname{tr} (S_E + \tilde{S})$ as a heat source, then we can read (4.6) as the condition of balance of granular energy, *i.e.* as the granular heat transfer equation. Thus we can also compare (4.6) with (4) of [5], the identifications being straightforward; in particular, I , their local rate of dissipation of pseudo-energy, coincides with $-\operatorname{tr} \tilde{S}$.

We must still adapt to the continuum scheme the equation of balance of moment of

momentum (3.17). This goal can be achieved by requiring that total power of all internal actions vanish for all rigid virtual velocities. As, within the limits already mentioned, (not only the stir but also) the power $-(\text{grad } v) \cdot T$ generated in the macro motion is transferred to the motion of agitation, but for the term $\text{tr } \tilde{S}$, we need only require that

$$(4.7) \quad -\text{tr}(\text{div } \mathbf{S}) + \text{tr } \tilde{S} = 0,$$

for all rigid velocity fields. This condition restricts the type of constitutive laws that can be proposed for \mathbf{S} and \tilde{S} , very much as happens in the classical case with the requirement that T be symmetric.

5. COMPARISON WITH A THEORY OF FAST FLOWS OF GRANULAR MATERIALS

As already mentioned, there are analogies between our final proposal of extended balance equations and the celebrated results of Grad's 13-moment theory, especially when they are read as adapted by Jenkins *et al.* for the analysis of fast flows of granular materials. There remain difficulties in comparing (4.5) with the contracted form of (32) in [1] (see also (43) in [1]); however, that last equation was not given, so far, a decisive rôle in explicit applications.

Actually, Jenkins' approach is much more fruitful than ours, in that it allows one to deduce also specific constitutive relations for H and S ; an essential step, which is missing here. Thus we conclude by at least transcribing in our notation the constitutive prescriptions from [1] and [2].

In [1] we find (see p. 373) that the classical relations must apply for T and q

$$(5.1) \quad T = -(p - \omega \text{div } v)I + 2\mu \text{dev grad } v, \quad q = -\kappa \text{grad } \theta;$$

besides

$$\text{tr } \tilde{S} = \varepsilon \theta.$$

In addition, appropriate specifications of the dependence on other quantities or explicit values must apply for p , ω , μ , κ , ε (see (68), (66), (69), (72) and (79) of [1]).

In [2] the deduced constitutive laws are

$$(5.2) \quad \begin{cases} T = -\rho H, & \mathbf{S}_{ijk} = \frac{2}{5} (q_i \delta_{jk} + q_j \delta_{ki} + q_k \delta_{ij}), \\ q = \beta M^{-1} (3H(\text{grad } \theta) + 2(\text{grad } H)H), \end{cases}$$

where

$$M = d_0 I + d_1 \text{dev } H + d_2 (\text{dev } H)^2 - 9a \text{sym grad } v - 5a \text{skw grad } v$$

with appropriate choices for the scalar coefficients.

It would be also interesting to extract, from [4] and papers on extended thermodynamics, alternative constitutive prescriptions; we restrict ourselves here to the remark that those prescriptions do not involve, on principle, gradients of the state variables, as happens instead in both (5.1) and (5.2)_{III}.

In closing we address the reader to the very recent paper [6] for an overview of the many issues involving granular materials.

Dedicated to the memory of our friend and teacher James F. Bell, who has often reminded theorists, and proved experimentally, that Nature does not always comply with their, though harmonious, fantasies.

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