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Inertia effects as a possible missing link between micro and macro second-order work in granular media

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This paper is concerned with a theoretical question as to the definition of instabilities in a granular assembly and its proper formulation at the microscopic level. Recently, this question has taken up much prominence with the emergence of intriguing failure modes such as diffuse failure associated to unstable plasticity of granular materials and microstructural instabilities. An analysis of the second-order work as a general and necessary criterion to detect instabilities is conducted both at the macroscopic and microscopic levels including large deformations. On the basis of a micromechanical analysis of a body consisting of arbitrary interacting particles in a representative element volume (REV), a general formula is derived to quantify the microscopic second-order work involving local variables on the grain scale. The latter emerges as a sum of a configurational term that involves contact forces between neighboring grains, plus a kinetic part consisting of the mechanical unbalance of intergranular forces under dynamics at incipient failure. The present analysis is thought to serve as a clarification of the question of failure in geomaterials typified by a transition from static to a dynamic regime with release of kinetic energy originating from microstructural interactions.

1. Introduction

The theoretical study of instabilities in random heterogeneous media has proved to be an interesting pursuit in the development of a proper continuum framework for defining instability in geomaterials. Its influence transcends the scales down to the micro level and extends beyond applications that are being herein contemplated. In this present work, we are specifically interested in establishing a linkage between macroscopic and microscopic instabilities and their respective mathematical expressions through a theoretical analysis which bridges the two scales.

The microstructural investigation of instabilities has already received much attention in the past several years. While one of the ambitions was to elucidate which basic microstructural aspects lead to a macroscopic instability, a prime obstacle is the diversity in the definition of the notion of instability, as highlighted in Bagi (2007). According to the definition proposed by Bagi, which is in line with Lyapunov's definition, an equilibrium mechanical state of a given material system is considered unstable if its kinetic energy increases in a finite way under an infinitesimal load increase

(disturbance). This increase in kinetic energy corresponds to a transition (which is basically a bifurcation¹) from a quasi-static regime toward a dynamical one (Nicot et al., 2009; Darve et al., 2007; Daouadji et al., 2010). The dynamical regime is associated with a failure process that can be either diffuse or localized.

It is commonly acknowledged, with the exclusion of flutter instabilities, that a general and necessary condition for instability to occur in rate-independent materials is given by the so-called "second-order work criterion", which corresponds to the loss of positive definiteness of the elasto-plastic tangent constitutive matrix (Hill, 1958; Bigoni and Hueckel, 1991; Petrick, 1993; Challamel et al., 2010; see also experimental contributions of Lade: Lade and Pradel, 1990; Lade, 1992). More specifically, excluding flutter instabilities, a necessary and sufficient condition is that (see for instance Nicot et al., 2011):

- The equilibrium state belongs to the bifurcation domain, in which the symmetric part of the tangent constitutive operator admits at least one negative eigenvalue. Indeed, the boundaries of the bifurcation domain are given by the surface where the

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¹ A bifurcation can be defined as a discontinuous change in the response of a given system, under a continuous evolution of both state and loading variables. Other definitions can also be found in the literature.

determinant of that symmetric part of the constitutive operator vanishes first and by the plastic limit condition (vanishing of the constitutive determinant itself). Inside this domain, loading directions exist along which the second-order work takes negative values.

- The loading is controlled by mixed parameters, some being composed of stress components, while the others of strain components.
- The mixed control parameters impose a loading direction associated with a negative value of the second-order work.

In non-associated plasticity, it turns out that the elasto-plastic matrix is non-symmetric and as such, the emerging bifurcation domain is bounded by an outer surface given by the plastic limit condition and an inner surface defined by the first vanishing values of the determinant of the symmetric part of the constitutive matrix (Darve et al., 2004; Nicot et al., 2007a; Wan et al., 2011). Within such a bifurcation domain, the second order work lends itself to the detection of a variety of unstable states involving either plastic strain localization or diffuse deformation (Nicot and Darve, 2011b). In this context, the second order work plays a fundamental role in the analysis of divergence instabilities not only in geomechanics (by virtue of geomaterials being intrinsically non-associated), but also in structural mechanics where the stiffness matrix is non-symmetric due to non-conservative or dissipative forces (Challamel et al., 2010). Viewed at the macroscopic level where a representative elementary volume (REV) is invoked, the second-order work can be computed as the inner product of the Piola–Kirchhoff incremental stress tensor and the spatial gradient of the incremental displacement.

Moreover, the microstructural origin of the existence of an unstable state and the dynamical regime that ensues (depending on the loading conditions) is thought to be linked to the stability of elementary grain assemblies at an intermediate, mesoscopic scale (Kuhn and Chang, 2006; Tordesillas and Muthuswamy, 2009; Tordesillas et al., 2010), including both cluster patterns of grains (n -grains cycles) and linear patterns (force chains). The stability of these patterns directly depends upon the possible relative motion of each grain, and therefore on the constitutive behavior on the contact scale (Kuhn and Chang, 2006; Valanis and Peters, 1996; Bazant and Cedolin, 1991).

From the above discussion, it becomes clear that a proper local variable that can be related to the macroscopic second-order work is needed as an indicator of local stability. Along these lines, a discrete definition of second-order work was proposed by Nicot and Darve (2007) at the microscopic level (i.e. the grain level), by involving local microstructural variables such as the inter-granular incremental force and the inter-granular incremental displacement at a contact point.

The objective of this paper is to discuss whether there is a connection between macroscopic second-order work and the sum of microscopic second-order work contributions from all grain contacts inside the REV so as to establish a general framework relating second-order work to microstructure. According to previous numerical investigations based on the discrete element method (DEM) reported in Nicot et al. (2007b, 2009), it appears that replacing the macroscopic second-order work with the sum of all individual microscopic second-order works in a REV is only valid when deformations are small (this is the case, for example, when all contacts behave elastically). As soon as large deformations appear in the system, the above two do not agree anymore since important microstructural rearrangements develop, associated in general with outbursts in kinetic energy.

In order to elucidate such a difference between the macroscopic second-order work and the sum of individual microscopic second-order works, a theoretical analysis of basic notions of stress and material description in a body consisting of interacting particles

is first presented. After recalling Lagrangian and Eulerian formulations of the macroscopic second-order work (Section 2), we finally elaborate the microscopic counterparts (Section 3). Following a micromechanical analysis, the difference between expressions of the second-order work at the two scales is attributed to the local unbalance of interparticle forces due to local dynamic effects induced by local granular avalanches occurring in the plastic deformation regime.

Throughout this paper, time and spatial derivatives of any variable ψ will be distinguished by denoting $\delta\psi$ the time differentiation of ψ (defined as the product of the particulate derivative $\dot{\psi}$ and the infinitesimal time increment δt) with respect to a given reference frame, and by denoting $d\psi$ the spatial differentiation of ψ , with $d\psi = (\partial\psi/\partial x_i)d x_i$. For any (first- or second-order) tensor A , A^t denotes the transpose tensor. In addition, the developments expounded in this work pertain to large strains.

2. Instability, kinetic energy and second-order work

As one of the main positions taken in the introduction, a material point at a given mechanical (stress–strain) state during loading history is eminently unstable if loading conditions exist such that a transition from a quasistatic regime to a dynamical occurs with an increase in kinetic energy. Hence, in this section, the link between the increase in kinetic energy and the second-order work is reviewed.

Consider a material body of volume V_0 enclosed by boundary (Γ_0) in an initial configuration C_0 so as to describe its motion under external loading in an incremental formulation. Following a certain loading history, the body is in a strained configuration C and occupies a volume V of boundary (Γ) , in equilibrium under a prescribed external loading. This loading is controlled by specific static or kinematic parameters, referred to as the control parameters.

Let the transformation χ associating each material point \bar{x} of the current configuration C with a corresponding material point \bar{X} of the initial configuration C_0 be introduced such that $\bar{x} = \chi(\bar{X})$. The continuity of matter ensures that the map χ is bijective. Then, any field $f(\bar{x})$ of the current positions \bar{x} can be transformed into a field $\tilde{f}(\bar{X}) = f(\bar{x})$ of the initial positions. When no confusion is possible \bar{X} , the notation “ \sim ” will be omitted. Since the map χ is bijective, the Jacobian J of the tangent linear transformation \bar{F} is strictly positive, with the latter being a function of the positions \bar{X} and $\tilde{F}_{ij} = \partial x_i / \partial X_j$. The displacement field $\bar{u}(\bar{x})$ of material points \bar{x} between both initial and current configurations is defined by the relation $\bar{x} = \chi(\bar{X}) = \bar{X} + \bar{u}(\bar{x}) = \bar{X} + \bar{\tilde{u}}(\bar{X})$.

The current configuration C at time t is considered to be an equilibrium state. Thus, both the kinetic energy and its rate for the material system in the current configuration C are zero. The second-order time differentiation of the kinetic energy written in Lagrangian description (Nicot et al., 2007a; Nicot and Darve, 2007) is:

$$\delta^2 E_c(t) = \int_{V_0} \delta f_i \delta \tilde{u}_i dS_0 - \int_{V_0} \delta \Pi_{ij} \frac{\partial(\delta \tilde{u}_i)}{\partial X_j} dV_0 \quad (1)$$

where $\bar{\Pi}$ is the first Piola–Kirchhoff stress tensor and \bar{f} the current forces applied to the initial (reference) configuration. Eq. (1) introduces explicitly the second-order work which following a semi-Lagrangian formalism (Hill, 1958) is expressed as:

$$W_2 = \int_{V_0} \delta \Pi_{ij} \delta \tilde{F}_{ij} dV_0; \delta \tilde{F}_{ij} = \frac{\partial(\delta x_i)}{\partial X_j} = \frac{\partial(\delta u_i)}{\partial X_j} \quad (2)$$

Despite the Lagrangian description being a natural way of following the motion of particles of the system, an Eulerian description can also be envisaged. Thus, the second-order work

formulated in Eulerian description will involve the Cauchy stress tensor $\bar{\sigma}$. Using the change in variables $\bar{x} = \chi(\bar{X})$, both $\bar{\sigma}$ and $\bar{\Pi}$ stress tensors are related through the Piola relation, i.e.

$$\bar{\Pi} = J \bar{\sigma} \left(\bar{F}^{-1} \right)^t \quad (3)$$

All terms in Eq. (3) are function of the positions \bar{X} and, upon differentiation and rearranging terms, yields:

$$\delta \bar{\Pi} = J \delta \bar{\sigma} \left(\bar{F}^{-1} \right)^t + \delta J \bar{\sigma} \left(\bar{F}^{-1} \right)^t - J \bar{\sigma} \left(\bar{F}^{-1} \right)^t \left(\delta \bar{F} \right)^t \left(\bar{F}^{-1} \right)^t \quad (4)$$

and finally gives:

$$\delta \bar{\sigma} = \frac{1}{J} \delta \bar{\Pi} \left(\bar{F} \right)^t - \frac{\delta J}{J} \bar{\sigma} + \frac{1}{J} \bar{\Pi} \left(\delta \bar{F} \right)^t \quad (5)$$

When the two configurations C_0 and C coincide at time t (as in an updated Lagrangian description), $\bar{\Pi} = \bar{\sigma}$, $\bar{F} = \bar{I}$ and $J = 1$. However, as the current configuration C will evolve from time t , $\delta \bar{F} \neq 0$ and $\delta J \neq 0$. Due to the updating of configurations, Eq. (4) simplifies into:

$$\delta \bar{\Pi} = \delta \bar{\sigma} + \frac{\delta J}{J} \bar{\sigma} - \bar{\sigma} \left(\delta \bar{F} \right)^t = \delta \bar{\sigma} + \frac{\delta J}{J} \bar{\Pi} - \bar{\Pi} \left(\delta \bar{F} \right)^t \quad (6)$$

or

$$\delta \bar{\sigma} = \delta \bar{\Pi} - \frac{\delta J}{J} \bar{\Pi} + \bar{\Pi} \left(\delta \bar{F} \right)^t \quad (7)$$

As expected in an Eulerian formulation where the boundaries of the material body change continuously, the incremental Cauchy stress tensor in Eq. (7) is composed of three terms:

- $\delta \bar{\Pi}$ accounting for the change in forces acting in a fixed configuration,
- $-(\delta J/J) \bar{\Pi}$ accounting for the change in the bulk volume, and
- $\bar{\Pi} (\delta \bar{F})^t$ related to the change in the geometrical configuration under constant forces.

Finally, substituting Eq. (4) into Eq. (2), the second-order work expressed in terms of Cauchy stress is given by

$$W_2 = \int_{V_0} J \left(\delta \bar{\sigma} + \frac{\delta J}{J} \bar{\sigma} - \bar{\sigma} \left(\bar{F}^{-1} \right)^t \left(\delta \bar{F} \right)^t \right) \left(\bar{F} \right)^t : \delta \bar{F} dV_0 \quad (8)$$

Recalling that for any matrices \bar{A} , \bar{B} and \bar{C} :

$$\bar{A} : (\bar{B} \bar{C}) = (\bar{A} \bar{C}^t) : \bar{B} = (\bar{B}^t \bar{A}) : \bar{C} \quad (9)$$

Eq. (8) can be rewritten as:

$$W_2 = \int_{V_0} \left(\delta \bar{\sigma} + \frac{\delta J}{J} \bar{\sigma} - \bar{\sigma} \left(\delta \bar{F} \bar{F}^{-1} \right)^t \right) : \delta \bar{F} \bar{F}^{-1} J dV_0 \quad (10)$$

It is worth noting that:

$$\delta \bar{F}_{ij} = \frac{\partial(\delta \tilde{u}_i)}{\partial X_j} = \frac{\partial(\delta u_i)}{\partial x_k} \frac{\partial x_k}{\partial X_j} = L_{ik} \tilde{F}_{kj} \delta t \quad (11)$$

which gives:

$$\bar{L} \delta t = \delta \bar{F} \bar{F}^{-1} \quad (12)$$

where $\bar{L} = \partial(\dot{\bar{u}})/\partial \bar{x}$ is the velocity gradient tensor, function of current positions \bar{x} .

Then, using the change in variables $\bar{X} = \chi^{-1}(\bar{x})$, and recalling that $dV = J dV_0$, the integral in Eq. (10) can be expressed in the current configuration, leading to the Eulerian expression of the second-order work:

$$W_2 = \int_V \left(\delta \bar{\sigma} + \frac{\delta J}{J} \bar{\sigma} - \bar{\sigma} \left(\bar{L} \right)^t \delta t \right) : \bar{L} \delta t dV \quad (13)$$

It should be noted that the expression of the second-order work takes a straightforward form when applied to a material point. Indeed, if homogeneous conditions exist in volume V , recalling that $\delta J = J \delta V/V$, Eq. (13) simply becomes:

$$W_2 = V \left(\left(\delta \bar{\sigma} + \frac{\delta V}{V} \bar{\sigma} \right) : \bar{L} \delta t - \bar{\sigma} \left(\bar{L} \right)^t : \bar{L} (\delta t)^2 \right) \quad (14)$$

When the two configurations C_0 and C coincide at time t (updated Lagrangian configuration), $\bar{L} \delta t = \delta \bar{F}$, and Eq. (14) reads as:

$$W_2 = V \left(\left(\delta \bar{\sigma} + \frac{\delta V}{V} \bar{\sigma} \right) : \delta \bar{F} - \bar{\sigma} \left(\delta \bar{F} \right)^t : \delta \bar{F} \right) \quad (15)$$

Noting the symmetry of the Cauchy stress tensor, Eq. (15) can also be rewritten as:

$$W_2 = V \delta \bar{\sigma} : \bar{D} \delta t + \delta V \bar{\sigma} : \bar{D} \delta t - V \bar{\sigma} \left(\delta \bar{F} \right)^t : \delta \bar{F} \quad (16)$$

where $\bar{D} = (\bar{L} + \bar{L}^t)/2$.

An important consequence of Eq. (16) is that the standard expression $W_2 = V \delta \bar{\sigma} : \bar{D} \delta t$ is generally not valid.

By contrast, the absence of geometrical effects is a great advantage of the Lagrangian description since the motion is formulated with respect to a fixed configuration, leading to a straightforward expression of the second-order work in homogeneous conditions, i.e.

$$W_2 = V \delta \Pi_{ij} \frac{\partial(\delta \tilde{u}_i)}{\partial X_j} = V \delta \Pi_{ij} \delta \tilde{F}_{ij} \quad (17)$$

In the following, an updated Lagrangian configuration will be adopted: the current configuration stands as the reference configuration, $\bar{\Pi} = \bar{\sigma}$, $\bar{F} = \bar{I}$ and $J = 1$.

3. The second-order work as a link between micro and macro scales

The problem at hand is now specialized into a homogeneous volume of granular material comprised of N grains (the homogeneity refers here to the material properties of grains, as well as to the texture – or fabric – of the granular assembly). Throughout the paper, ‘ p ’ will denote indiscriminately the grain (as a body) or enumerate a particular grain within the assembly such that $1 \leq p \leq N$. The shape of each grain ‘ p ’ is arbitrary. At a given time t , each grain ‘ p ’ is in contact with n_p other grains ‘ $q \in \{p_k\}$ ’ with $k = 1, \dots, n_p$, whereas the total number of contacts at this time t within the assembly is denoted N_c . Boundary particles, belonging to the boundary ∂V , are distinguished from internal ones occupying volume $V = V - \partial V$ strictly inside the boundary.

The system is assumed to be in equilibrium at a given time t under a prescribed external loading. Depending on the type of loading control, each grain ‘ p ’ belonging to the boundary ∂V of the considered volume is subjected to either a displacement (kinematic control) or an external force $\bar{f}^{ext,p}$ (static control), possibly zero.

3.1. The stress tensor

The transmission of forces in granular materials operates at contacts of adjoining grains, thereby resulting into a macroscopic average stress at the grain ensemble level. There, we find that the stress tensor in such a body of volume in equilibrium under external forces $\bar{f}^{ext,p}$ applied to the boundary particles ‘ p ’ of position \bar{x}^p can be defined by the classical Love–Weber formula (Love, 1927; Weber, 1966; Christoffersen et al., 1981; Mehrabadi et al., 1982), i.e.

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in \partial V} f_i^{\text{ext},p} x_j^p \quad (18)$$

It is useful to transform the above expression in order to introduce the inter-particle contact forces \bar{f}^c such that (see Appendix A):

$$\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} f_i^c l_j^c + \frac{1}{V} \sum_{p \in V} f_i^p x_j^p \quad (19)$$

where \bar{l}^c is the branch vector relating the centers of contacting particles, and \bar{f}^p denotes the resultant force applied to the particle 'p'. In the absence of inertial effects or when all particles are in static equilibrium, the second term in Eq. (19) vanishes. However, this term may subsist in the presence of internal dynamical effects that arise from local force unbalances, even if the whole granular body may be in equilibrium macroscopically. In this connection, we present in what follows the latter general case.

The summation of a given contact variable ψ^c over all existing contacts at a given time t can be written in the form:

$$\sum_{c=1}^{N_c} \psi^c = \sum_{p=1}^N \sum_{k=1}^{n_p} \psi^{p,p_k} \quad (20)$$

If the quantity $\psi^{p,q}$ is set to zero for any pair of particles 'p' and 'q' not in contact, then it is useful to rewrite Eq. (20) as:

$$\sum_{c=1}^{N_c} \psi^c = \sum_{p=1}^N \sum_{q=1}^p \psi^{p,q} = \sum_{p,q} \psi^c \quad (21)$$

where the symbol $\sum_{p,q}$ signifies the summation over p and q varying over $[1, N]$ with $q \leq p$, and c refers to the contacting pair (p, q) . The benefit of using the form of Eq. (21) is that all summations involve indices p and q varying over a fixed range. Then, the differentiation of term $\sum_{p,q} \psi^c$ is simply given by

$$\delta \left(\sum_{p,q} \psi^c \right) = \sum_{p,q} \delta \psi^c \quad (22)$$

In the Eulerian formulation represented in Eq. (19), the contact forces, the branch vectors, the location of each particle and the volume of the specimen are bound to evolve over a given loading history from an initial configuration $C_0(\bar{f}_0^c, \bar{l}_0^c, \bar{x}_0^c, V_0)$. Thus, referring to the initial configuration, the analogous form of the stress tensor in Lagrangian description is:

$$\Pi_{ij} = \frac{1}{V_0} \sum_{p,q} f_i^c l_{0,j}^c + \frac{1}{V_0} \sum_{p \in V_0} f_i^p x_{0,j}^p \quad (23)$$

The differentiation of Eq. (19), at a given time t , yields:

$$\begin{aligned} \delta \sigma_{ij} = & \frac{1}{V} \sum_{p,q} \delta f_i^c l_j^c - \frac{\delta V}{V} \sigma_{ij} + \frac{1}{V} \sum_{p,q} f_i^c \delta l_j^c + \frac{1}{V} \sum_{p \in V} \delta f_i^p x_j^p + \frac{1}{V} \\ & \times \sum_{p \in V} f_i^p \delta x_j^p \end{aligned} \quad (24)$$

which when identified with Eq. (6) and noting $\delta J = J(\delta V/V)$ leads to:

$$\begin{aligned} \frac{1}{V} \left(\sum_{p,q} f_i^c \delta l_j^c + \sum_{p,q} \delta f_i^c l_j^c + \sum_{p \in V} \delta f_i^p x_j^p + \sum_{p \in V} f_i^p \delta x_j^p \right) \\ = \frac{1}{J} \left(\Pi_{ik} \delta \bar{F}_{jk} + \delta \Pi_{ik} \bar{F}_{jk} \right) \end{aligned} \quad (25)$$

We recall that the Lagrangian stress tensor $\bar{\Pi}$ is by definition computed from the current forces with respect to the fixed and undeformed initial configuration. Thus, the time rate of change of $\bar{\Pi}$ is found from differentiation of Eq. (23) as:

$$\delta \Pi_{ij} = \frac{1}{V_0} \sum_{p,q} \delta f_i^c l_{0,j}^c + \frac{1}{V_0} \sum_{p \in V_0} \delta f_i^p x_{0,j}^p \quad (26)$$

If at time t both initial and current configurations coincide (such as in a so-called updated Lagrangian setting) $\bar{l}^c = \bar{l}_0^c$, $\bar{x}^p = \bar{x}_0^p$, $\bar{V} = \bar{V}$, and $J = 1$. Eq. (23) becomes:

$$\delta \Pi_{ij} = \frac{1}{V} \sum_{p,q} \delta f_i^c l_j^c + \frac{1}{V} \sum_{p \in V} \delta f_i^p x_j^p \quad (27)$$

Eq. (25) taken together with the above Eq. (27), and by virtue of Eq. (23), gives:

$$\begin{aligned} \frac{1}{V} \left(\sum_{p,q} f_i^c \delta l_j^c + \sum_{p \in V} f_i^p \delta x_j^p \right) = \Pi_{ik} \delta \bar{F}_{jk} \\ = \frac{1}{V} \left(\sum_{p,q} f_i^c \delta \bar{F}_{jk} l_k^c + \sum_{p \in V} f_i^p \delta \bar{F}_{jk} x_k^p \right) \end{aligned} \quad (28)$$

Although the above treatment pertains to a general case where there may exist local interparticle force unbalances, we focus attention here on the special case these local unbalances may be neglected ($f_i^p = 0$) so as to gain some insights in Eq. (28). Then, by making $i = j$, and summing up on the repeated indices, we obtain:

$$\frac{1}{V} \sum_{p,q} f_i^c \delta l_i^c = \Pi_{ik} \delta \bar{F}_{ik} = \frac{1}{V} \sum_{p,q} f_i^c \delta \bar{F}_{ik} l_k^c \quad (29)$$

In the above, we note that the scalar product $f_i^c (\delta l_i^c - \delta \bar{F}_{ik} l_k^c)$ summed over all contacts vanishes even though the quantity $(\delta l_i^c - \delta \bar{F}_{ik} l_k^c)$ is not zero (locally, the change in the branch vectors within a specimen does not derive from a unique tensor; Cambou et al., 2000; Agnolin and Krut, 2008; Agnolin and Roux, 2008). We also observe that the term on the right hand side of Eq. (29) refers to the incremental strain energy within the volume V . Interestingly, the left hand side term does not work out to be the work done by contact forces, given that the scalar product involves the branch vector, and not the relative displacement between a pair of contacting particles.

3.2. A microscopic formulation of the second-order work

The second-order work, as defined in Eq. (15) or (17), refers to a quantity related to macroscopic entities of a system of interacting point masses (material points) or discrete particles. In the specific case of granular materials, it is of interest to express the second-order work with respect to microscopic variables to appropriately account for the microstructure of the material. To this end, the micromechanical derivation of the stress tensor presented in the previous section constitutes a sound basis.

Recalling that $(\delta J/J) = (\delta V/V)$, time differentiation of Eq. (25) gives:

$$\begin{aligned} \frac{1}{V} \left(\sum_{p,q} \delta^2 f_i^c l_j^c + 2 \sum_{p,q} \delta f_i^c \delta l_j^c + \sum_{p,q} f_i^c \delta^2 l_j^c + \sum_{p \in V} \delta^2 f_i^p x_j^p + 2 \sum_{p \in V} \delta f_i^p \delta x_j^p + \sum_{p \in V} f_i^p \delta^2 x_j^p \right) \\ = \frac{1}{J} \left(\delta^2 \Pi_{ik} \bar{F}_{jk} + 2 \delta \Pi_{ik} \delta \bar{F}_{jk} + \Pi_{ik} \delta^2 \bar{F}_{jk} \right) \end{aligned} \quad (30)$$

Furthermore, if at time t both initial and current configurations coincide, making $i = j$ and summing over repeated indices, it follows that:

$$\begin{aligned} \sum_{p,q} \delta^2 f_i^c l_i^c + 2 \sum_{p,q} \delta f_i^c \delta l_i^c + \sum_{p,q} f_i^c \delta^2 l_i^c + \sum_{p \in V} \delta^2 f_i^p x_i^p + 2 \sum_{p \in V} \delta f_i^p \delta x_i^p \\ + \sum_{p \in V} f_i^p \delta^2 x_i^p = V \delta^2 \Pi_{ij} + 2V \delta \Pi_{ij} \delta \bar{F}_{ij} + V \Pi_{ij} \delta^2 \bar{F}_{ij} \end{aligned} \quad (31)$$

Recalling Eq. (27), the time differentiation of the incremental Lagrangian stress tensor $\delta \bar{\Pi}$ can be formally written as:

$$\delta^2 \Pi_{ij} = \frac{1}{V} \sum_{p,q} \delta^2 f_i^c \delta l_j^c + \frac{1}{V} \sum_{p \in V} \delta^2 f_i^p \delta x_j^p \quad (32)$$

Substitution of Eqs. (23) and (32) into (31) and noting that $W_2 = V \delta \Pi_{ij} \delta \tilde{F}_{ij}$, lead to the second-order work relationship:

$$W_2 = \sum_{p,q} \delta f_i^c \delta l_i^c + \sum_{p \in V} \delta f_i^p \delta x_i^p + \frac{1}{2} \sum_{p,q} f_i^c \left(\delta^2 l_i^c - \delta^2 \tilde{F}_{ij} l_j^c \right) + \frac{1}{2} \sum_{p \in V} f_i^p \left(\delta^2 x_i^p - \delta^2 \tilde{F}_{ij} x_j^p \right) \quad (33)$$

which can be transformed by replacing the summation over all contacts with a summation over particles. Thus, the term $\sum_{p,q} f_i^c \delta^2 l_i^c$ can be expressed as:

$$\sum_{p,q} f_i^c \delta^2 l_i^c = \frac{1}{2} \sum_{p=1}^N \sum_{q=1}^N f_i^{p,q} \delta^2 l_i^{p,q} \quad (34)$$

where $\tilde{f}^{p,q}$ denotes the force applied by the particle 'p' onto the particle 'q', and $\tilde{l}^{q,p}$ the branch vector connecting particle 'q' to particle 'p'. When there is no contact between particles 'p' and 'q', then $\tilde{f}^{p,q}$ is obviously zero.

Since $l_i^{p,q} = (x_i^p - x_i^q)$ and $f_i^{p,q} = -f_i^{q,p}$, Eq. (34) simplifies into:

$$\sum_{p,q} f_i^c \delta^2 l_i^c = - \sum_{p \in V} \left(\left(\sum_{q \in V} f_i^{q,p} \right) \delta^2 x_i^p \right) \quad (35)$$

For an internal particle 'p', $\sum_{q \in V} \tilde{f}^{q,p}$ represents the resultant force \tilde{f}^p applied by the adjoining particles to the particle 'p'. For a boundary particle 'p', $\tilde{f}^p = \sum_{q \in \partial V} \tilde{f}^{q,p} + \tilde{f}^{ext,p}$. Thus, Eq. (35) becomes:

$$\sum_{p,q} f_i^c \delta^2 l_i^c = - \sum_{p \in V} f_i^p \delta^2 x_i^p + \sum_{p \in \partial V} f_i^{ext,p} \delta^2 x_i^p \quad (36)$$

Similarly:

$$\sum_{p,q} f_i^c \delta^2 \tilde{F}_{ij} l_j^c = - \sum_{p \in V} f_i^p \delta^2 \tilde{F}_{ij} x_j^p + \sum_{p \in \partial V} f_i^{ext,p} \delta^2 \tilde{F}_{ij} x_j^p \quad (37)$$

It then follows that:

$$\begin{aligned} & \sum_{p,q} f_i^c \left(\delta^2 l_i^c - \delta^2 \tilde{F}_{ij} l_j^c \right) + \sum_{p \in V} f_i^p \left(\delta^2 x_i^p - \delta^2 \tilde{F}_{ij} x_j^p \right) \\ &= \sum_{p \in \partial V} f_i^{ext,p} \left(\delta^2 x_i^p - \delta^2 \tilde{F}_{ij} x_j^p \right) \end{aligned} \quad (38)$$

As such, the second-order work in Eq. (33) is reduced to:

$$W_2 = \sum_{p,q} \delta f_i^c \delta l_i^c + \sum_{p \in V} \delta f_i^p \delta x_i^p + \frac{1}{2} \sum_{p \in \partial V} f_i^{ext,p} \left(\delta^2 x_i^p - \delta^2 \tilde{F}_{ij} x_j^p \right) \quad (39)$$

Assuming that the loading engenders macro-homogeneous strain and stress fields within the specimen in the sense given by Hill (1967), the incremental displacement of a material point of position \bar{X} belonging to the boundary ∂V of the volume is a homogeneous function of degree one with respect to the position \bar{X} , so that:

$$\delta \tilde{u}_i = \delta x_i = \frac{\partial(\delta \tilde{u}_i)}{\partial X_j} X_j = \delta \tilde{F}_{ij} X_j \quad \text{and} \quad \delta^2 \tilde{u}_i = \delta^2 x_i = \delta^2 \tilde{F}_{ij} X_j \quad (40)$$

When both initial and current configurations coincide, $\bar{X} = \bar{x}$ with:

$$\delta x_i = \delta \tilde{F}_{ij} x_j \quad \text{and} \quad \delta^2 x_i = \delta^2 \tilde{F}_{ij} x_j \quad (41)$$

It must be emphasized that Eq. (41) hold for boundary particles only. The incremental displacement of internal particles deviates from the affine prediction associated with the gradient tensor $\delta \tilde{F}$. Thus, the following basic relation is derived from Eq. (39):

$$W_2 = \sum_{p,q} \delta f_i^c \delta l_i^c + \sum_{p \in V} \delta f_i^p \delta x_i^p \quad (42)$$

Eq. (42) shows that the micromechanical expression of the second-order work is the combination of two terms.

The first term $\sum_{p,q} \delta f_i^c \delta l_i^c$ involves both contact forces and branch vectors between adjoining grains. As branch vectors connect the centers of adjoining grains, this first term depends on the internal particle topology (packing). It can be regarded therefore as a configurational term. The second term $\sum_{p \in V} \delta f_i^p \delta x_i^p$ of Eq. (42) introduces the incremental unbalanced force $\delta \tilde{f}^p$ applied to each particle 'p'. When inertial effects are small (in quasi-static regime for example), the contribution of this term becomes negligible too. However, when rapid particles motions occur, this term is likely to be no longer negligible. This finding explains why in discrete element simulations, replacing the macroscopic second-order work with the sum of all individual microscopic second-order works in a REV is valid only in quasistatic regime. This simplification fails as soon as rapid microstructural rearrangements occur, such as the opening of contacts in the plastic regime, as demonstrated in Nicot et al. (2007b).

It should be noted that the term $\delta f_i^c \delta l_i^c$ can be related to the microscopic second-order work $W_2^c = \delta f_i^c \delta u_i^c$ related to a given contact 'c' (Nicot and Darve, 2007; Nicot et al., 2007b). If \tilde{f}^c is the force applied by the particle 'p' onto the particle 'q', $\tilde{l}^c = \bar{x}^p - \bar{x}^q$ is the branch vector pointing from particle 'q' to particle 'p', and $\delta \tilde{u}^c$ is the relative displacement of a particle 'p' with respect to a particle 'q' (see Fig. 1). Since:

$$\begin{aligned} \delta \tilde{u}^c &= \delta \tilde{u}^p - \delta \tilde{u}^q + \tilde{r}^{q,p} \wedge \delta \tilde{\omega}^q - \tilde{r}^{p,q} \wedge \delta \tilde{\omega}^p \\ &= \delta \tilde{l}^c + \tilde{r}^{q,p} \wedge \delta \tilde{\omega}^q - \tilde{r}^{p,q} \wedge \delta \tilde{\omega}^p \end{aligned} \quad (43)$$

it follows that:

$$\delta \tilde{f}^c \cdot \delta \tilde{u}^c = \delta \tilde{f}^c \cdot \delta \tilde{l}^c - (\tilde{r}^{q,p} \wedge \delta \tilde{f}^{p,q}) \cdot \delta \tilde{\omega}^q - (\tilde{r}^{p,q} \wedge \delta \tilde{f}^{q,p}) \cdot \delta \tilde{\omega}^p \quad (44)$$

which implies:

$$\begin{aligned} W_2^c &= \sum_{p,q} \delta f_i^c \delta l_i^c \\ &= \sum_{p,q} \left((\tilde{r}^{q,p} \wedge \delta \tilde{f}^{p,q}) \cdot \delta \tilde{\omega}^q + (\tilde{r}^{p,q} \wedge \delta \tilde{f}^{q,p}) \cdot \delta \tilde{\omega}^p \right) \end{aligned} \quad (45)$$

As a consequence, in the absence of particle rotation, the microscopic second-order work reduces to $\delta f_i^c \delta l_i^c$. In that case:

$$W_2 = \sum_{p,q} W_2^c + \sum_{p \in V} \delta f_i^p \delta x_i^p \quad (46)$$

As seen in Eq. (17), the macroscopic second-order work is the inner product between the incremental Piola-Kirchhoff tensor and the tangent linear transformation. Both incremental terms are related through the constitutive relation. For this reason, the second-order work for a material point has the mathematical structure of a

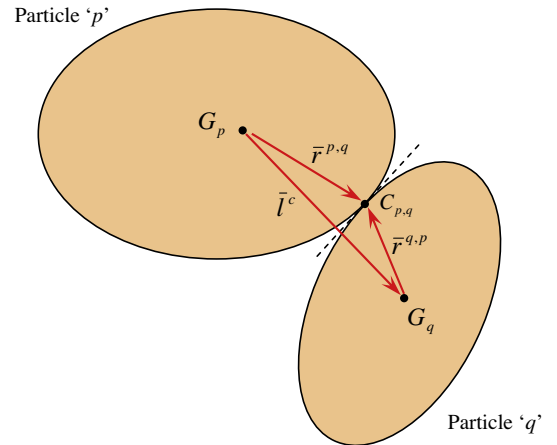


Fig. 1. Particles in contact. Geometrical description.

quadratic form associated with the constitutive operator at this material point (see for instance Nicot et al., 2009, 2010). The properties of the second-order work (vanishing) are therefore intimately related to the constitutive properties of the material. By the same token, the term $W_2^c = \delta f_i^c \delta u_i^c$ refers to the microscopic second-order work, because it is actually a quadratic form associated with the local constitutive behavior at the contact scale. Indeed, as both incremental contact forces δf_i^c and relative displacements δu_i^c are related through a constitutive relation $\delta f_i^c = k_{ij}^c \delta u_j^c$, where k_{ij}^c is the local constitutive operator, the product $\delta f_i^c \delta u_i^c$ leads to $k_{ij}^c \delta u_i^c \delta u_j^c$. The algebraic features of this quadratic form, with respect to the constitutive properties of the local constitutive operator, were extensively investigated in a series of papers (Nicot and Darve, 2006, 2007).

One of the main achievements of this investigation, through Eq. (42), is to shed light on the role played by the term $\delta f_i^c \delta l_i^c$ in the micromechanical definition of the second-order work. As appeared in Eq. (42), this micromechanical definition introduces explicitly the term $\delta f_i^c \delta l_i^c$, and not the term $\delta f_i^c \delta u_i^c$, even though both are connected as discussed above. This is a rather counter intuitive result since the product $W_2^c = \delta f_i^c \delta u_i^c$ seems to have the same mathematical structure as that of the macroscopic second-order work. Furthermore, Eq. (42) constitutes the micromechanical expression of the second-order work that also enables a microstructural investigation of the vanishing of the second-order work, a basic and necessary condition for failure to occur (Darve et al., 2004; Nicot et al., 2009, 2010). It is desirable to analyze such a derived micro-macro second-order work relationship with a micromechanical model to investigate the findings put forth in the first place. In the past, such a micromechanical model was proposed (Nicot and Darve, 2005) with some limitations arising from a too restrictive kinematic localization scheme which assumes an affine projection of macro- to micro-kinematics. The purpose of a future work consists in exploring the validity of the derived micro-macro second-order work relationship by using a newly-developed H -microdirectional model (Nicot and Darve, 2011a). In this model, the description of kinematics is enriched by introducing an intermediate scale (at a mesoscopic level) which implicates a periodic granular structure within which grains are arranged in a hexagonal pattern. Details of this mesoscopic treatment can be found in Nicot and Darve (2011a). A further step will consist of microstructural analyses derived from numerical computations based on a discrete element method, to track down how a granular mass organizes itself (likely through an intimate interplay between both the so-called weak and strong phases) during a failure process.

4. Concluding remarks

Various formulations of the second-order work in discrete granular media have been presented at differing scales to highlight the dominant role of microstructure when approaching failure. Starting from the basic Love-Weber formula that relates the (Cauchy or Piola-Kirchoff) stress tensor to local static variables and a proper description of kinematics of deformations in a granular assembly, the second-order work emerges as the sum of a configurational term involving both contact forces and branch vectors between adjoining grains (depending therefore on the internal particle topology), plus a kinetic term involving unbalanced forces between grains that arise from the dynamical nature of the material response at impending failure. Especially when the kinematics of the considered granular body is not controlled on its boundary (the incremental displacement of each boundary particle is not imposed), inertial phenomena may still occur inside the assembly. The mechanical unbalance of internal grains may result in dynamic effects marking failure of the body. When these dynamic effects related to microstructural rearrangements are negligible, then the second-order work merely

reduces to the configurational term (sum of the scalar products of the contact forces and the branch vectors over all the contacts). Otherwise, the dynamic counterpart has to be accounted for in the micromechanical expression of the second-order work.

As the vanishing of the second-order work is believed to be a relevant indicator of an unstable state for the material (Nicot et al., 2009), the derived expression should be useful in the better understanding of microstructural mechanisms that occur within a granular assembly in an unstable state, and during the phases leading to the failure of the material (Tordesillas, 2007; Tordesillas and Muthuswamy, 2009; Tordesillas et al., 2010).

This investigation opens new perspectives in the understanding of the key mechanisms leading to the failure of granular specimens. Numerical simulations based on both a micromechanical model and a discrete element method are now in progress in order to examine the influence of the internal inertial mechanisms on the macroscopic destabilization of granular bodies.

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Appendix A

The Love-Weber formula gives the macroscopic stress tensor within a REV of volume containing N particles in equilibrium under the external forces $\bar{f}^{ext,p}$ applied to the boundary particles 'p' of position \bar{x}^p :

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in \partial V} f_i^{ext,p} x_j^p \quad (A1.1)$$

For each particle 'p' of the REV, the resultant force \bar{f}^p can be expressed as:

$$\bar{f}_i^p = \sum_{q \in V} f_i^{q,p} + f_i^{ext,p} \quad (A1.2)$$

where $\bar{f}^{p,q}$ denotes the contact force between both particles 'p' and 'q' (force exerted by particle 'p' onto 'q'). When these particles are not in contact, then $\bar{f}^{p,q}$ vanishes. In addition, for particles belonging to the inner volume (excluding the boundary volume), $\bar{f}^{ext,p}$ is zero as well. Thus:

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in V} f_i^{ext,p} x_j^p \quad (A1.3)$$

Starting with Eq. (A1.2), it follows that:

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in V} f_i^p x_j^p - \frac{1}{V} \sum_{p \in V} \sum_{q \in V} f_i^{q,p} x_j^p \quad (A1.4)$$

Noting that $\sum_{p \in V} \sum_{q \in V} f_i^{q,p} x_j^p = \sum_{q \in V} \sum_{p \in V} f_i^{p,q} x_j^q$ (by interchanging 'p' with 'q'), and $\bar{f}^{p,q} = -\bar{f}^{q,p}$, we get:

$$\sum_{p \in V} \sum_{q \in V} f_i^{q,p} x_j^p = - \sum_{p \in V} \sum_{q \in V} f_i^{p,q} x_j^q = \frac{1}{2} \sum_{p \in V} \sum_{q \in V} f_i^{q,p} (x_j^p - x_j^q) \quad (A1.5)$$

Finally,

$$\sigma_{ij} = \frac{1}{V} \sum_{p \in V} f_i^p x_j^p + \frac{1}{2} \sum_{p \in V} \sum_{q \in V} f_i^{q,p} (x_j^p - x_j^q) \quad (A1.6)$$

The term $\frac{1}{2} \sum_{p \in V} \sum_{q \in V} f_i^{q,p} (x_j^p - x_j^q)$ represents the summation over all the N_c contacts 'c' between two adjoining particles 'p' and 'q' of the product $f_i^c l_j^c$, where $f_i^c = f_i^{q,p}$ and $l_j^c = x_j^p - x_j^q$. The alternate form

of the Love–Weber formula, involving internal contact forces, can therefore be derived, i.e.

$$\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} f_i^c l_j^c + \frac{1}{V} \sum_{p \in V} f_i^p x_j^p \quad (\text{A1.7})$$

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