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The effects of particle dynamics on the calculation of bulk stress in granular media

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ABSTRACT

Expressions for bulk stress within a granular material in a dynamic setting are reviewed and explicitly derived for assemblies of three dimensional arbitrary shaped particles. By employing classical continuum and rigid body mechanics, the mean stress tensor for a single particle is separated into three distinct components; the familiar Love–Webber formula describing the direct effect of contacts, a component due to the net unbalanced moment arising from contact and a symmetric term due to the centripetal acceleration of material within the particle. A case is made that the latter term be ignored without exception when determining bulk stress within an assembly of particles. In the absence of this centripetal term an important observation is made regarding the nature of the symmetry in the stress tensor for certain types of particles; in the case of particles with cubic symmetry, the effects of dynamics on the bulk stress in an assembly is captured by an entirely skew-symmetric tensor. In this situation, it is recognised that the symmetric part of the Love–Webber formula is all that is required for defining the mean stress tensor within an assembly – regardless of the dynamics of the system.

1. Introduction and background

In recent times the homogenisation processes involved in developing a continuous, macroscopic definition of stress in a discrete granular material have received a great deal of attention. At one level the definition of stress is quite straight-forward and generally uncontested, however the area has spawned its fair share of historical debate. Most of this debate surrounded the potential for asymmetry in the stress tensor (Bardet and Vardoulakis, 2001; Bagi, 2003; Kuhn, 2003; Bardet and Vardoulakis, 2003a,b; Froiio et al., 2006) and arguments for the existence of 'couple stresses' in the granular continuum (Chang et al., 1990; Oda, 1999; Oda et al., 2000; Ehlers et al., 2003; Ehlers, 2010; Alonso-Marroquin, 2011; Goldhirsch, 2010). This is now largely resolved with general acceptance that, without contact moments, asymmetry does not exist in equilibrium (de Saxcé et al., 2004; Fortin et al., 2003). Some recent work has even demonstrated that asymmetry is not necessarily inherent in the presence of contact moments, provided such moments are properly accounted for in the homogenisation process (Wensrich, 2014).

The majority of prior work has focused on material in equilibrium or in a quasi-static state. Here a variety of approaches have been used such as the mean stress theorem as initially applied by Love (1927) and Weber (1966), course graining (e.g. Goldhirsch, 2010; Edwards and Grinev, 1999; Weinhart et al., 2012) and variational methods (i.e. virtual work, Bardet and Vardoulakis, 2001; Chang et al., 2005; Mehrabadi et al., 1982; Christoffersen et al., 1981; Satake, 1983; Goddard, 2007). From the perspective of these static approaches, apparent asymmetry can arise if the assumption of equilibrium is violated. In response there has been a significant amount of recent work focused on developing consistent homogenisation processes that are applicable even in the absence of equilibrium. These approaches largely focus on calculating stress as an ensemble average of the stress within individual particles, defined from the point of view of the conservation of momentum at all points within a given particle (de Saxcé et al., 2004; Fortin et al., 2003; Fortin et al., 2002; Li et al., 2009; Nicot et al., 2013; Moreau, 2010; Luding, 2010). This work has shown that the components of stress arising from particle dynamics may be significant and are necessary for eliminating the asymmetry present in earlier quasi-static descriptions.

In this paper, we apply a similar approach to define stress within a dynamic granular assembly as an ensemble average over individual particles subject to the laws of classical continuum theory and rigid body mechanics. For the most part, the approach taken here is known (de Saxcé et al., 2004; Fortin et al., 2003; Fortin et al., 2002; Li et al., 2009; Nicot et al., 2013; Moreau,

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2010; Luding, 2010), however we consider three-dimensions and arbitrary particle shape and progress to the point where a new interpretation can be made. In particular, we present an argument that the component of stress relating to the angular velocity of particles, often referred to as "centrifugal stress" (de Saxcé et al., 2004; Nicot et al., 2013), be excluded without exception from the definition of bulk stress. Without this term, we make further observations on the nature of stress symmetry in granular materials that will greatly simplify the process of accounting for dynamics in certain classes of materials, including the vast majority of Discrete Element Models where spherical particles are still commonplace.

2. Bulk stress in the absence of equilibrium

As has been discussed many times in the literature (e.g. Drescher and do Josselin de Jong, 1972), the basic definition of Cauchy stress within a granular assembly usually relies on a volume average over a suitable Representative Volume Element, V_{RVE};

$$\langle\sigma\rangle = \frac{1}{V_{RVE}}\int_{V_{RVE}} \sigma dV \tag{1}$$

This volume average represents the average stress within a continuous domain corresponding to the discrete assembly of particles. By considering the stress within each particle separately, it is possible to express this average as;

$$\langle\sigma\rangle = \frac{1}{V_{RVE}}\sum_{P\in V_{RVE}} V^P\langle\sigma^P\rangle, \tag{2}$$

where $\langle\sigma^p\rangle$ is the volume average of stress within particle 'P', with volume V^P. With this in mind, we proceed with the rest of our analysis focused on the stress within a single particle – the above definition will allow us to relate this to bulk averages. This also applies for any time-volume or weighted time-volume averaging methods (e.g. Babic, 1997; Zhu and Yu, 2002).

Consider the particle shown in Fig. 1. This particle is subject to boundary tractions, $\{\tilde{\tau}^c\}$, via contact with other particles in the assembly, body force densities due to actions such as gravity, $\tilde{\gamma}$, and is not necessarily in equilibrium. At any point within the particle the conservation of momentum implies that;

$$\nabla\sigma + \tilde{\gamma} = \rho\ddot{\tilde{x}}, \tag{3}$$

where $\ddot{\tilde{x}}$ is the total derivative of velocity at the point in question.

Relying on the Gauss–Qstrogradsky divergence theorem, it can then be shown (e.g. Nicot et al., 2013) that the mean stress within the particle can be written;

$$\langle\sigma^p\rangle = \frac{1}{V^p}\left(\sum_c \int_{A^c} \tilde{\tau}^c\otimes\tilde{x}dA - \int_{V^p}\left(\rho\ddot{\tilde{x}} - \tilde{\gamma}\right)\otimes\tilde{x}dV\right), \tag{4}$$

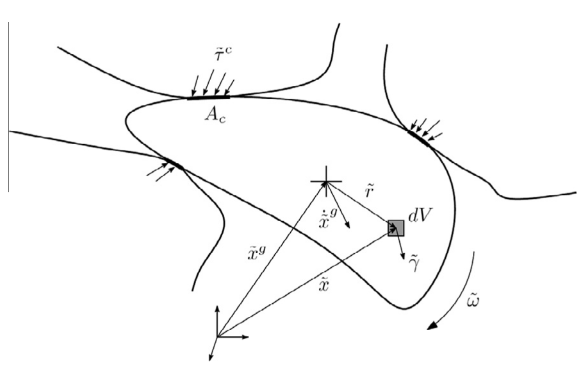

Fig. 1. A single particle forming a part of a granular assembly is subject to a number of contact traction forces, $\{\tilde{\tau}^c\}$, and a body force density, $\tilde{\gamma}$.

where the symbol $\otimes$ represents the dyadic product between vectors.

If we assume that the particle is rigid we can characterise the contact tractions as a set of discrete forces, $\left\{\tilde{f}^c = \int_{A^c}\tau^c dA\right\}$, acting at corresponding contact points $\{\tilde{x}^c\}$. Together with an assumption that the particles are homogeneous and subject to a constant body force density, Eq. (4) becomes;

$$\langle\sigma^p\rangle = \frac{1}{V^p}\sum_c \tilde{f}^c\otimes\tilde{x}^c - \frac{1}{V^p}\rho\int_{V^p}\ddot{\tilde{x}}\otimes\tilde{x}dV + \frac{1}{V^p}\tilde{\gamma}\otimes\int_{V^p}\tilde{x}dV \tag{5}$$

Thus the stress within the particle can be represented by the sum of three distinct components. For future reference, we identify them as follows;

$$\langle\sigma^p\rangle_{Lw} = \frac{1}{V^p}\sum_c \tilde{f}^c\otimes\tilde{x}^c, \tag{6}$$

is the familiar 'Love–Webber' formula (Love, 1927; Weber, 1966) describing the stress due to the contact forces;

$$\langle\sigma^P\rangle_I = -\frac{1}{V^P}\rho\int_{V^P}\ddot{\tilde{x}}\otimes\tilde{x}dV, \tag{7}$$

is an inertial component from the dynamics of the particle; and,

$$\langle\sigma^P\rangle_B = \frac{1}{V^P}\tilde{\gamma}\otimes\int_{V^P}\tilde{x}dV, \tag{8}$$

is that originating from the body forces.

The body force component can be easily simplified by expressing the position of points within the particle relative to the centre of mass, $\tilde{x} = \tilde{x}^g + \tilde{r}$, leading to;

$$\langle\sigma^P\rangle_B = \frac{1}{V^P}\tilde{\gamma}\otimes\int_{V^P}(\tilde{x}^g + \tilde{r})dV = \tilde{\gamma}\otimes\tilde{x}^g \tag{9}$$

As has been done recently by Nicot et al. (2013), we can analyse the inertial component from the perspective of the rigid body assumption by expressing the acceleration of any point within the particle as follows[1]

$$\ddot{\tilde{x}} = \ddot{\tilde{x}}^g + \dot{\tilde{\omega}}\times\tilde{r} + \tilde{\omega}\times(\tilde{\omega}\times\tilde{r}) \tag{10}$$

where $\tilde{\omega}$ is the angular velocity of the particle. Substituting this into the inertial component of stress we obtain the following;

$$\langle\sigma^P\rangle_i = -\rho\ddot{\tilde{x}}^g\otimes\tilde{x}^g - \frac{1}{V^P}\rho\int_{V^P}\left(\dot{\tilde{\omega}}\times\tilde{r}\right)\otimes\tilde{r}dV - \frac{1}{V^P}\rho\int_{V^P}(\tilde{\omega}\times(\tilde{\omega}\times\tilde{r}))\otimes\tilde{r}dV \tag{11}$$

With the aid of the vector triple product rule; $\tilde{a}\times(\tilde{b}\times\tilde{c}) = \tilde{b}(\tilde{a}\cdot\tilde{c}) - \tilde{c}(\tilde{a}\cdot\tilde{b})$ Eq. (11) can be written;

$$\langle\sigma^P\rangle_I = -\rho\ddot{\tilde{x}}^g\otimes\tilde{x}^g - \frac{1}{V^P}\rho\int_{V^P}\left(\dot{\tilde{\omega}}\times\tilde{r}\right)\otimes\tilde{r}dV - \frac{1}{V}\rho\int_{V^P}(\tilde{\omega}\cdot\tilde{r})\tilde{\omega}\otimes\tilde{r}dV + \frac{1}{V^P}\rho\int_{V^P}(\tilde{\omega}\cdot\tilde{\omega})\tilde{r}\otimes\tilde{r}dV, \tag{12}$$

or in component form;

$$\langle\sigma^P_{ij}\rangle_I = -\rho\ddot{\tilde{x}}^g_i\tilde{x}^g_j - \frac{1}{V^P}\rho\int_{V^P}\varepsilon_{ikl}\dot{\omega}_k r_l r_j dV - \frac{1}{V^P}\rho\int_{V^P}\omega_l r_l\omega_i r_j dV + \frac{1}{V^P}\rho\int_{V^P}\omega_k\omega_k r_i r_j dV, \tag{13}$$

where ε_{ijk} is the usual Levi–Civita permutation symbol.

[1] Due to the rigid body assumption, we have not explicitly written Eq. (3) in terms of convected derivatives (as has been done previously by Luding (2010)). In this instance, the effects of rotation within the material are captured by Eq. (10).

Without loss of generality, we set the origin of our coordinate system so that $\tilde{x}^g = \tilde{0}$. By writing the second moment of mass tensor for the particle as $\mu_{ij} = \rho \int_{V^p} r_i r_j dV$, Eq. (13) then becomes;

$$\langle \sigma^p_{ij} \rangle_I = \frac{1}{V^P}\left(-\varepsilon_{ikl}\dot{\omega}_k \mu_{lj} - \omega_l \omega_i \mu_{lj} + \omega_k \omega_k \mu_{ij}\right). \tag{14}$$

Note that μ has been referred to as the 'inertia tensor' (Nicot et al., 2013) or the 'planar inertia tensor' (Moreau, 2010), however it should not be confused with the usual moment of inertia tensor that describes the rotational inertia of a rigid body. Obviously these two tensors are related.

Nicot et al. (2013) proceeded from this point to examine the behaviour of spherical (and circular) particles where the second moment and inertia tensors can be represented by scalars in constant ratio to each other. In this simplified system, the dynamic components were shown to consist of a skew-symmetric term related to the moment imbalance and a symmetric term related to the angular velocity of particles.

In a more general sense, we can examine the nature of arbitrary shaped particles by recognising that the second moment of mass is related to the usual moment of inertia tensor by the following;

$$I_{ij} = \mu_{kk}\delta_{ij} - \mu_{ij} \tag{15}$$

Again without loss of generality, we are free to choose a coordinate system that aligns with the principal directions of the particle.[2] In such a coordinate system the second moment and inertia tensors both appear diagonal and we can expand the index notation in Eq. (14) to yield the following expression for the inertial component of stress;

$$\langle \sigma^p_{ij} \rangle_i = \frac{1}{V^p}\begin{bmatrix} (\omega_2^2+\omega_3^3)\mu_{11} & -(\omega_1\omega_2-\dot{\omega}_3)\mu_{22} & -(\omega_1\omega_3+\dot{\omega}_2)\mu_{33} \\ -(\omega_2\omega_1+\dot{\omega}_3)\mu_{11} & (\omega_1^2+\omega_3^2)\mu_{22} & -(\omega_2\omega_3-\dot{\omega}_1)\mu_{33} \\ -(\omega_3\omega_1-\dot{\omega}_2)\mu_{11} & -(\omega_3\omega_2+\dot{\omega}_1)\mu_{22} & (\omega_1^2+\omega_2^2)\mu_{33} \end{bmatrix} \tag{16}$$

From Euler's equation of motion, we can express the components of angular acceleration of the particle in terms of the net (unbalanced) moment, $\tilde{M}$, as;

$$\begin{aligned} \dot{\omega}_1 &= \frac{M_1 + (\mu_{33}-\mu_{22})\omega_2\omega_3}{\mu_{22}+\mu_{33}} \\ \dot{\omega}_2 &= \frac{M_2 + (\mu_{11}-\mu_{33})\omega_1\omega_3}{\mu_{11}+\mu_{33}} \\ \dot{\omega}_3 &= \frac{M_3 + (\mu_{22}-\mu_{11})\omega_1\omega_2}{\mu_{11}+\mu_{22}} \end{aligned} \tag{17}$$

Substitution into Eq. (16) provides the following expression for the dynamic components of stress;

$$\begin{aligned} \langle \sigma^P \rangle_i = {} & \frac{1}{V^P}\begin{bmatrix} 0 & \frac{M_3\mu_{22}}{\mu_{11}+\mu_{22}} & \frac{-M_2\mu_{33}}{\mu_{11}+\mu_{33}} \\ \frac{-M_3\mu_{11}}{\mu_{11}+\mu_{22}} & 0 & \frac{M_1\mu_{33}}{\mu_{22}+\mu_{33}} \\ \frac{M_2\mu_{11}}{\mu_{11}+\mu_{33}} & \frac{-M_1\mu_{22}}{\mu_{22}+\mu_{33}} & 0 \end{bmatrix} \\ & + \frac{1}{V^P}\begin{bmatrix} (\omega_2^2+\omega_3^2)\mu_{11} & -\frac{2\mu_{11}\mu_{22}}{\mu_{11}+\mu_{22}\omega_1\omega_2} & -\frac{2\mu_{11}\mu_{33}}{\mu_{11}+\mu_{33}}\omega_1\omega_3 \\ -\frac{2\mu_{11}\mu_{22}}{\mu_{11}+\mu_{22}}\omega_1\omega_2 & (\omega_1^2+\omega_3^2)\mu_{22} & -\frac{2\mu_{22}\mu_{33}}{\mu_{22}+\mu_{33}}\omega_2\omega_3 \\ -\frac{2\mu_{11}\mu_{33}}{\mu_{11}+\mu_{33}}\omega_1\omega_3 & -\frac{2\mu_{22}\mu_{33}}{\mu_{22}+\mu_{33}}\omega_2\omega_3 & (\omega_1^2+\omega_2^2)\mu_{33} \end{bmatrix} \end{aligned} \tag{18}$$

The first term in this expression relates to the component of stress that is due to any net moment that may be applied to the particle (i.e. the rate of change of angular momentum). Given that we have assumed a constant body force density, the sole remaining source for this net moment is through the contact forces and is of the form;

$$\tilde{M} = \sum_c \tilde{r}^c \times \tilde{f}^c \tag{19}$$

The second term in Eq. (18) is symmetric and relates to the centripetal acceleration of material within the particle. This component depends directly on the particle's angular velocity and is akin to the average tensile stress experienced within a rotating flywheel (note that the hydrostatic component of this term is always positive). This component is not related to contact or body forces in any direct way.

3. The case for a new definition for granular stress

Following explicitly from the definition provided in Eq. (1), Eqs. (5) and (18) describe a bulk stress made up of 4 individual components;

(1) The familiar Love–Webber equation that directly captures the effects of the contact forces,
(2) The effects of body forces,
(3) The effects of rotational inertia, expressed in terms of the net moment arising from contacts, and,
(4) The effects of centripetal acceleration within the particles.

The first two relate to static effects where-as the latter originate from dynamics. It should be noted that a similar dissection of stress has been made previously by others; notably by Nicot et al. for the case of spheres and disks (Nicot et al., 2013) as well as Moreau (2010). As was demonstrated by Nicot et al., the dynamic terms are significant and necessary for symmetry; however neither Nicot et al. nor Moreau further distinguished between the two dynamic components in terms of their physical relevance in the granular continuum. We will now draw this distinction.

The first three components characterise the effects of external actions applied to the particles (i.e. contact forces, unbalanced moments, and body forces). These actions directly influence the motion of particles and those that surround them. The last is distinctly different in this sense. It provides a tensile stress in response to internal (centripetal) actions within the particle; it has no direct relationship with external actions, nor does it have any effect on the overall state of the system. To illustrate this point, consider the case of a number of non-contacting particles floating in space with non-zero angular velocities (e.g. asteroids). Strict application of Eq. (18) would lead to the conclusion that this 'assembly' of particles is experiencing a non-zero hydrostatic tensile stress – a curious interpretation indeed!

From this perspective, there is a reasonable case to be made that the centripetal term in Eq. (18) should not be considered part of the bulk stress in the equivalent granular continuum. It is required for the conservation of momentum within the particle, but is entirely unrelated to the conservation of momentum in the assembly outside. Without this term, the three remaining components of bulk stress directly relate to forces and moments experienced by the particles rather than internal actions within them.

Note that we are not arguing that this component of stress does not exist. On the contrary, it is possible to imagine a scenario where this component may contribute to the breakage of particles if angular velocities are high enough. However, we are pointing out that, short of this extreme situation, it has no impact on the behaviour

[2] We should be mindful that the average over the RVE is performed in a global coordinate system that will not necessarily align with the principal directions of any particle in the assembly. However, we can be confident that all conclusions that will be drawn in principal directions will be preserved through any necessary coordinate transformations into a global system.

of the assembly overall. It should also be noted that we are not implying that centripetal effects are not present in the assembly as a whole. Centripetal effects during bulk rotation of an assembly of grains would have a direct impact on the bulk stress via the contact forces necessary for that motion to occur. We are arguing for the omission of centripetal effects within particles, not centripetal effects as experienced by the material in bulk form (as described by the conservation of momentum for the continuum).

4. Symmetry of stress in a dynamic setting

With the origin placed at the centre of mass, the stress from the body forces is zero. Neglecting the centripetal term, the two remaining components of stress are the Love–Webber equation describing the effect of the contact forces and the inertial component describing the effect of the unbalanced moment. As has been discussed at length in the literature (e.g. Bardet and Vardoulakis, 2001; Bagi, 2003; Kuhn, 2003; Bardet and Vardoulakis, 2003a,b; Froiio et al., 2006; de Saxcé et al., 2004; Fortin et al., 2003), any appropriate expression for bulk stress should provide a symmetric tensor. Together with Eq. (19), we can observe this directly by calculating the asymmetric part of our remaining two terms;[3]

$$\langle \sigma^P_{[ij]} \rangle = \frac{1}{2V^P}\left(\varepsilon_{ijk}M_k + \sum_c \left(f^c_i r^c_j - f^c_j r^c_i\right)\right) = 0 \tag{20}$$

We can extend this observation by noting that in some circumstances the remaining inertial component is entirely skew-symmetric. If we consider particles whose geometry has cubic symmetry[4] (e.g. spheres, cubes, octohedra, and many other irregular polyhedra etc.) we can write $\mu_{11} = \mu_{22} = \mu_{33}$, and the resulting expression for granular stress becomes;

$$\langle \sigma^P_{ij} \rangle = \frac{1}{V^P}\sum_c f^c_i r^c_j + \frac{1}{2V^P}\varepsilon_{ijk}M_k \tag{21}$$

Given that the inertial term in Eq. (21) is skew-symmetric, it takes no part in forming the symmetric part of this expression. From this we can draw the conclusion that the resulting mean stress tensor can be calculated precisely as the symmetric portion of the Love–Webber equation. In particular, this result implies that the symmetric part of the Love–Webber equation is all that is required for the calculation of granular stress in the vast majority of Discrete Element Models where spherical particles are still commonplace. No special accounting for dynamics (other than the removal of asymmetry) is necessary in these systems. Strictly speaking, if cubic symmetry is not present (e.g. DEM using oblate/prolate spheroids or general polyhedra), the stress tensor should include an additional component as defined by the (non-zero) symmetric portion of the first term in Eq. (18). The magnitude of which is governed by the magnitude of unbalanced moments acting on the particle and level of departure from cubic symmetry.

It is also worth mentioning that this result has been demonstrated in the absence of contact moments such as rolling friction which have become a general feature of many DEM simulations (e.g. Ai et al., 2011; Wensrich and Katterfeld, 2012; Wensrich et al., 2013). Without careful scrutiny, contact moments can appear to introduce additional asymmetry into the Love–Webber equation, however, as mentioned earlier, this asymmetry has been recently demonstrated to be artifactual through the concept of contact eccentricity (Wensrich, 2014). With this work in mind, the conclusions we have drawn here should be thought to apply to all spherical systems even in the presence of contact moments. This is provided that any contact moments are represented by contact eccentricities as was outlined in this prior work.

[3] Note that the centripetal term is clearly symmetric; its removal has no impact on the symmetry of the resulting expression.

[4] Cubic symmetry is marked by 90° rotational symmetry/invariance in any direction.

5. Conclusions

Following from the usual definition of bulk stress as a volume average over a representative volume, the mean stress tensor within a granular assembly has been derived from the point of view of classical continuum theory. Assuming the particle is rigid, homogenous and subject to point contact forces, we have demonstrated that the mean stress tensor can be separated into two distinct components; the familiar Love–Webber formula and an inertial component due to particle dynamics. By considering the mechanics of the particles as separate rigid bodies, the dynamic component of stress has been further separated into two parts; a component expressed in terms of the net moment arising from contact and a symmetric term arising from the centripetal acceleration of material within the particle. A reasonable case has been made that the latter of these components represents internal actions within the individual particles and should be omitted from the definition of ‘bulk stress’ within a granular assembly.

At a fundamental level, the conservation of angular momentum implies that any reasonable definition of stress should provide a symmetric tensor. We have explicitly shown that this is guaranteed here, even in the case of a dynamic system. Together with prior work demonstrating the existence of symmetry even in the presence of contact moments, the case for the existence of ‘couple stresses’ in granular materials is becoming more difficult.

It was further noted that if the particles within an assembly possess cubic symmetry (common in many DEM simulations) the component of stress arising from the net moments applied to the particle is entirely skew-symmetric. The conclusion we draw from this is that the stress tensor calculated by considering the detailed dynamics of the assembly is identical to the symmetric component of the Love–Webber equation. It should be noted that, without specific justification, it is quite common for stress to be calculated as the symmetric part of the Love–Webber equation, as is done in many numerical studies. From this point of view, the present work could be viewed as explicit support for existing approaches; however this support only extends to particles with cubic symmetry.

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