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Mesoscale investigation of fine grain contribution to contact stress in granular materials

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Abstract: Fine grains play an important role in mechanical properties of granular materials as they control how plastic strain may develop, which has a noticeable impact on mechanical stability. In this work, we use numerical simulations based on a discrete element method (DEM) to analyze the stress contribution of fine grains to the total stress. Different from usual DEM simulations, the analysis is conducted directly at the mesoscopic scale by considering an idealized grain assembly. The results show how fine grains get progressively jammed and increasingly participate to stress transmission. Fine contribution to contact stress is shown to be non-isotropic. The principal anisotropy direction coincides with the principal direction of contraction and the anisotropy ratio (i.e. the ratio between the largest and the smallest eigenvalues of the fine stress) is shown to be limited ($\sigma_{\text{max}}/\sigma_{\text{min}} \approx 2$). By performing strain controlled directional analyses, an analytical model is proposed to account for the stress contribution of fine grains along various loading paths. Its simple form will help to enrich
advanced micro-mechanically-based constitutive formulations, and better account for the constitutive behavior of widely graded granular materials.

**Keywords:** Granular material, Fine grains, DEM, Multiscale approach, Mesoscopic scale, contact stress, jamming.

**Introduction**

Granular materials are commonly found in nature (e.g. sands, rock or floating ice) as well as in industrial applications (e.g. drugs and chemicals). Despite an apparent simplicity, granular materials exhibit complex mechanical behavior and physical characteristics resulting from the collective reorganization of large numbers of grains of various shapes and sizes. In the field of soil mechanics, granular materials are made of grains of very different sizes, and the grain size distribution of such materials span over several orders of magnitude. If granular materials result from the mixture of two size of grains (such as for instance sand-silt mixture), we may split the grains into two classes, namely coarse and fine grains\(^1\) (Thevanayagam et al. 2002). The mass proportion of fine grains (usually named fine content or simply FC) has a significant effect on the mechanical properties of grain assemblies, and the role of fine grains in mixtures has received an acute attention in the literature (Lade and Yamamuro 1997; Monkul and Ozden 2007; Papadopoulou and Tika 2008; Cabalar 2011; Jiang et al. 2015; Zhou et al. 2018; Rahman et al. 2011; Shi et al. 2019; Shi et al. 2021; Thevanayagam et al. 2002; Cao et al. 2021; Ng et al. 2017; Zhou et al. 2018; Wang et al. 2021; Ueda et al. 2011). From a numerical point of view, discrete element methods (DEM) stand as an interesting tool to access to detailed and extensive information at grain scale level and improve the understanding of the mechanical role of fine grains in granular materials (Ahmadi et al. 2020; Gong and Liu 2017; Gong et al. 2019a and 2019b). For instance, DEM simulations showed that fine grains exhibit a smaller effective stress

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\(^1\) Note that in this paper, fine grains do not refer to particles smaller than 80 µm. Fine is used as opposed to coarse and only cohesionless materials, in which physico-chemical forces can be neglected, are considered here.
than coarse grains in gap-graded materials with low fine contents (Shire and O’Sullivan 2013; Shire et al. 2014). By artificially removing some fine grains in DEM simulations, some authors explored at the representative elementary volume (REV) scale the consequences on the mechanical behavior along triaxial loading paths (Scholtès et al. 2010; Hicher 2013; Zhang et al. 2019). By performing directional analyses, it was shown that the loss of fine grains modifies the microstructure which may be responsible for mechanical strength (Vallejo 2001; Deng et al. 2017; Wautier et al. 2019). In particular, fine grains were shown to control strain hardening mechanisms as well as the non-associated character of the flow rule in granular materials (Wautier et al. 2019; Wang et al. 2021). When considering internal erosion by suffusion, which corresponds to the selective erosion of the fine grains of a soil, assessing the failure potential of degraded hydraulic structures requires models in which the contribution of fine grains to the mechanical behavior is accurately modelled (Cui et al. 2017; Cui et al. 2019).

However, there is still a lack of constitutive models able to input microscale information and upscale the contribution of fine grains at the material point scale.

Different from DEM simulations at REV scale, the multiscale approach (Nicot and Darve 2005 and 2011; Yin et al. 2014; Wautier et al. 2021; Shi et al. 2020) provides an alternative way to derive constitutive behaviors from local contact laws and local grain rearrangements. This approach relies on an intermediate scale between contact scale and REV scale, namely the mesoscale. Instead of describing a REV of soil as a collection of a large number of grains, the multiscale approach uses a collection of independent mesostructures composed of a few grains. Multiscale models rely on statistical homogenization rather than spatial homogenization. The objective of such models is to define minimal assemblies of a few grains able to encapsulate the elementary mechanisms responsible for macroscopic behavior of granular materials. Consequently, multiscale models are able to incorporate microstructure information while keeping the computation cost much smaller than DEM simulations at REV scale.
Force chains (Radjai et al. 1998; Peters et al. 2005; Tordesillas 2007; Minh et al. 2014; Wautier et al. 2017; Liu et al. 2020) and grain loops (Zhu et al. 2016; Liu et al. 2018) are mesostructures that are recognized to govern the elementary mechanisms at stake in granular materials. Inspired by these granular material features, Nicot and Darve (2011) developed the H-model, in which an elementary mesostructure is proposed as a hexagonal grain loop combining two force chains in 2D. This model was successfully used at both REV and structure scales in several studies and confronted to experimental results (Xiong et al. 2019; Xiong et al. 2021; Wautier et al. 2021). The original dry cohesionless H-cell is composed of six grains of equal radii. Recently, Xiong et al. (2017, 2019) extended the H-model from 2D to 3D by building bi-hexagonal cells with ten grains of equal radii. Capillary effects can also be accounted for by adding a capillary stress tensor in the H-model (Xiong et al. 2021). However, until today, the H-cell has always been considered to be formed of grains of equal radii. Obviously, the particle size distribution (PSD) has an impact on the mechanical behavior of granular materials (Minh and Cheng 2013; Morgan 1999; Jiang et al. 2018; Liu et al. 2021). While it can easily be accounted for in DEM simulations at REV scale, it is difficult to account for any particle size distribution in an analytical multiscale model such as the H-model in which the mesostructure should be kept as simple as possible. As long as the particle size distribution of the considered materials is narrowly distributed, the H-model is relevant. However, it is clear that the H-model is not designed to deal with widely graded materials. As a first step, PSD of widely graded materials (or at least gap-graded materials) can be characterized by the size ratio between the largest and smallest grains, and by the fine content. As a result, the objective of this paper is to work on developing an enriched version of the H-model able to account for the presence of fine grains in the H-cell, in order to model (at least) gap-graded materials in under-filled regime (i.e. when coarse grains constitute the load-bearing skeleton).
To reach this objective, discrete element simulations are used in this study to compute the stress contribution of fine grains at the scale of an H-cell. A particular attention is paid to fine grain jamming mechanism, both through volumetric and shear deformation combinations. Compared with abundant literature on the physics of jamming in granular materials (Behringer and Chakraborty 2019; Bi et al. 2011; Majmudar et al. 2007; Tordesillas 2007; Wang et al. 2018; Luding 2016; Edwards and Grinev 2001), the novelty of the approach proposed in this study is to address the physics of jamming at mesoscale instead of the representative elementary volume scale, and to account for partial jamming/unjamming of the fine grains while coarse grains are kept in a jamming state. An analytical relationship for fine grain contribution to contact stress is derived in this paper from DEM data, which should pave the way for enriching the capabilities of the H-model.

The paper is organized as follows. The second section introduces the simulation process and the mechanical behavior of three-dimensional H-cells filled with fine grains is investigated along triaxial loading paths. Strain controlled directional analyses are conducted in the third section in a two-dimensional simplified framework to compute the stress contribution of fine grains to the stress. Eventually, an analytical model is derived in the fourth section to describe the stress contribution of fine grains at a mesoscopic scale.

**Mesoscale modelling of a bi-disperse material**

Different from more traditional studies dedicated to jamming in granular material, we propose here to investigate the jamming of fine grains in bi-disperse granular materials at the mesoscopic scale. To carry such analyses, there is a need to consider a mesostructure composed a few coarse grains in which fine grains are included. While the coarse grains are set in a jammed state from the very beginning, fine grains are inserted in an unjammed state. The jamming transition is tracked when the mesostructure is forced to deform. In this section,
qualitative results of the jamming process are shown in a particular set up in 3D conditions corresponding to the mesostructured of the 3D version of the H-model (Xiong 2017).

**DEM set up for the H-cell**

As an extension of the micro-directional model (Nicot and Darve 2005), the H-model was developed to describe the constitutive relation of granular materials by taking into account the local geometrical interactions between grains (Nicot and Darve 2011). In this model, the constitutive behavior of the soil results from the statistical averaging of the individual responses of a collection of elementary mesostructures composed of a few grains. The ten grains mesostructure used in the 3D H-model is shown in Fig. 1. It consists in two imbricated 2D H-cells, the geometry of which is given in Fig. 2.

![Fig.1 The mesostructure used in the 3D H-model (Xiong 2017)](image1)

![Fig.2 Mechanical description of one 2D H-cell (Xiong 2017)](image2)

As shown in Figure 2, the hexagonal geometry of the 2D H-cell is characterized by the opening angle $\alpha_1$ and the inter-granular distances $d_1$ and $d_2$. These parameters relate to the cell dimensions $l_1$ and $l_2$ as

$$
\begin{align*}
    l_1 &= d_2 + 2d_1 \cos \alpha_1 \\
    l_2 &= 2d_1 \sin \alpha_1
\end{align*}
$$

(1)
The distribution of external force (red) and force between particles in H-cell (blue) are shown in Figure 2 b) and c). In this study, the mechanical behavior of the 3D H-cell is simulated with the open source software LIGGGHTS (Kloss et al. 2012). The ten coarse grains in the H-cell are set to identical radius of 5 mm, while the initial opening angle $\alpha_1$ is set to 60°. Six boundary planes are added around the H-cell in order to control the cell deformation and measure the external contact forces shown in Figure 2.

Newton’s second law of motion governs the displacement of the grains interacting through the elasto-frictional contact law proposed by Cundall and Strack (1979).

Because the external walls are set frictionless in the DEM setup, the $G_2$ forces (see Figure 2) are set to zero in the simulations. To avoid subsequent grain rotations, the momentum balance equation is not solved for the coarse grains in the H-cell for which the degrees of freedom in rotation are blocked (Nicot and Darve 2011). As a result, the momentum balance equation will only apply to fine grains.

**Mesoscale simulation of coarse-fine mixture**

In order to simulate the response of a coarse-fine mixture at mesoscale, fine grains are randomly inserted into the inner volume of H-cell as illustrated in Figure 3 for two different grain size ratios. The particle size expansion method is adopted which enable to easily control the size ratio between the coarse and fine grains with different fine particle number as shown in Table 1.
Fig. 3 H-cells with fine grains for two size ratios: 10 on the left and 5 on the right.

Table 1 summarizes the different size ratios and fines number used in the following simulations while Table 2 lists the simulation parameters. Note that, in all cases, the fine grains are prepared in an unjammed state which explain why different fines number are considered. The selection of H-model parameters is based on the previous work (Xiong 2017, Xiong et al. 2019, Xiong et al. 2021), while the selection of particle size ratio and contact model in DEM is based on the previous work on suffusion (Zhou et al. 2020). The value of void ratio in Table 1 are calculated based on the inner domain of the H-cell highlighted in the Figure 4, which is surrounded by thick black lines. The definition of fines content in Table 1 is also based on this inner domain, the coarse content is corresponding to the fraction of the coarse grains included in this inner domain (the yellow part in Figure 4).

**Table 1** Description of the numerical cells used.

<table>
<thead>
<tr>
<th>Size ratio</th>
<th>Fines number</th>
<th>Void ratio of inner volume of the H-cell</th>
<th>Fines content (by mass)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1200</td>
<td>0.32</td>
<td>0.415</td>
</tr>
<tr>
<td></td>
<td>1000</td>
<td>0.41</td>
<td>0.371</td>
</tr>
<tr>
<td></td>
<td>800</td>
<td>0.53</td>
<td>0.321</td>
</tr>
<tr>
<td></td>
<td>600</td>
<td>0.66</td>
<td>0.258</td>
</tr>
<tr>
<td>5</td>
<td>110</td>
<td>0.48</td>
<td>0.342</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.53</td>
<td>0.321</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>0.63</td>
<td>0.274</td>
</tr>
</tbody>
</table>

**Table 2** H-cell initial geometry and grain scale parameters for the elasto-frictional contact law of Cundall and Strack (1979).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unit</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-cell initial opening angle</td>
<td>Degree</td>
<td>60</td>
</tr>
<tr>
<td>Coarse grains diameter (D)</td>
<td>mm</td>
<td>10</td>
</tr>
<tr>
<td>Grain density</td>
<td>kg/m³</td>
<td>2600</td>
</tr>
<tr>
<td>Contact normal rigidity (k_n/D)</td>
<td>GPa</td>
<td>5.0</td>
</tr>
<tr>
<td>Stiffness ratio (k_t/k_n)</td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>Contact friction angle</td>
<td>Degree</td>
<td>30</td>
</tr>
</tbody>
</table>

The effect of the fine grains on the mechanical response of an individual H-cell is explored along a drained triaxial loading path as shown in Figure 4. After the initial insertion of the fine grains in the inner part of H-cell, the consolidation of the specimen is obtained under a confining
pressure of 10 kPa. Then, the sample is compressed in the vertical direction at a constant strain rate while keeping the lateral stress constant. In order to avoid that the fine grains escape from the inner domain of the H-cell, virtual inner walls interacting only with the fine grains are added. Their position is based on the position of the center of the large grains (see Figure 4).

![Diagram](image)

**Fig.4** Mesoscale “drained triaxial test” on H-cells filled with fine grains. The inner domain of the H-cell is highlighted.

The stress-strain curves for different numbers of fine grains and size ratios are given in Figure 5. The bottom illustrations correspond to three representative points: the initial state, a state where fine grains participate to stress transmission and the state where the top and bottom large gains get into contact. The three illustrations on the left correspond to a fines number of 600 and a size ratio of 10, while the illustrations on the right correspond to a fines number of 80 and a size ratio of 5.
Fig. 5 Stress-strain curve under different fines number and size ratios. Bottom left illustrations correspond to 600 fine grains and a size ratio of 10, while the right illustrations correspond to 80 fine grains and a size ratio of 5.

The stress curves do not show much difference before the first peak ($\varepsilon_{zz} = 0.13$). After this point, fine grains get jammed which modifies the stress response.

In order to isolate the contribution of fine grains to the stress, the contact pairs (cp) can be sorted into three groups: coarse-coarse contacts (c-c), coarse-fine contacts (c-f) and fine-fine contacts (f-f). According to the Love-Weber formula (Love 2013; Mehrabadi et al. 1982), the contact stress can be decomposed as

$$
\sigma_{ij} = \frac{1}{V} \left( \sum_{cp \in c-c} f_i^{c-c} d_j^{c-c} + \sum_{cp \in c-f} f_i^{c-f} d_j^{c-f} + \sum_{cp \in f-f} f_i^{f-f} d_j^{f-f} \right)
$$

where $i$ and $j$ denote either $x$, $y$, or $z$, $f_i$ and $d_j$ represent the contact force and the branch vector connecting the centers of two contacting grains. By defining the mean pressure $p = \frac{1}{3} \sum_i \sigma_{ii}$ and the deviatoric stress $q = \sigma_{zz} - \sigma_{xx}$, $p$ and $q$ can be seen as the sum of mean pressure and deviatoric stress computed from c-c, c-f and f-f contacts as well. Figure 6 shows the stress
decomposition and the size of the contact populations for the triaxial loading with 600 fine grains and a size ratio of 10.

**Fig. 6** Evolution curves of stress and contact pair numbers (size ratio 10, fines number 600)

It can be observed that fine grains hardly contribute to the stress before a critical point around $\varepsilon_{zz} = 0.33$. Then fines get involved significantly in stress transmission and the number of c-f and f-f contacts rises.

The evolutions of the mean stress and the number contacts are shown in Figure 7 and Figure 8 for different numbers of fine grains. An abrupt activation transition is observed in the evolution of mean stress involving fines when the fines number is 600 and 800, while for a larger number of fine grains (Figure 7 (a, b)), a smoother activation occurring from the beginning of the deviatoric loading is observed.
Fig. 7 Mean stress evolution for different fines numbers: (a) 1200; (b) 1000; (c) 800; (d) 600

In Figure 8, such a development trend can be considered as the jamming behavior of frictional grains (Ciamarra et al. 2011) with a sharp rise in the coordination number and the stress level. Unclear jamming points are obtained when the fines number is 1000 and 1200, while a clear jamming point is detected for lower fines numbers.
Figure 8 provides a comparison between different coarse-fine size ratios with the same fine contents (same volume of fine grains). In both cases, a clear activation of the fine grains is visible. The coarse-fine size ratio has little effect on c-c and f-f contribution to the stress, but a larger contribution of c-f contacts is observed when coarse-fine size ratio is 5. Indeed, the increase in the size of the fine grains makes it more difficult for them to rearrange within the inner space of the H-cell without getting jammed. As a result, fine grains activate sooner during the vertical compression and are able to transmit larger stress levels when coarse-fine size ratio is smaller.
Fig.9 Mean stress decomposition according to the contact types for different coarse-fine size ratios (10 or 5). SZ refers to the coarse-fine size ratio, while CC, CF and FF refers to the contact type. For the two size ratios considered, the fine contents are the same (800 fine grains for SZ10 and 100 fine grains for SZ5).

2.3 A heuristic model for fine stress contribution

In the H-model, an analytical expression is derived from the contact stress resulting from coarse-coarse contact forces. Based on the contact stress definition proposed in Eq. (2), the effect of the fine grains can be isolated from the c-c contact stress and formally encapsulated in a matrix $\sigma_f$ as follows,

$$\sigma = \sigma^{c-c} + \sigma_f$$

$$\sigma_f = \frac{1}{V} \left( \sum_{cpe \in c-f} f^{c-f} \otimes d^{c-f} + \sum_{cpe \in f-f} f^{f-f} \otimes d^{f-f} \right)$$

Provided we have an explicit expression for this $\sigma_f$ matrix, the effect of fines can be readily implemented in the H-model: the fine stress adds to the meso-stress computed in the standard H-model.

As a first simple assumption, it is proposed to consider that i) fine grains get jammed when the inner volume of the H-cell become too small (isotropic jamming) and ii) once jammed, fine
grains behave as a compressible fluid inside the H-cell. Figure 10 illustrates this conceptual model. By adopting this modeling hypothesis, it is then possible to rewrite $\sigma_f$ as follows,

$$
\sigma_f = \begin{cases} 
0 & \text{if } V_{in} > V_{th} \\
K \frac{V_{th} - V_{in}}{V_{th}} & \text{if } V_{in} < V_{th}
\end{cases}
$$

where $V_{th}$ is the inner volume when fines get jammed (volume enclosed by the purple contour in Figure 10), $V_{in}$ is the current total inner volume in the H-cell not including the coarse grains ($V_{th}$ plus the light-yellow part in the Figure 10), and $K$ is a compressibility matrix. Should the proposed model be relevant, $K$ is expected to be proportional to the identity matrix with the proportionality coefficient being an isotropic compressibility modulus (hence the name compressibility matrix for $K$). In Eq. (4), $V_{th}$ is set as the reference point to evaluate the effects of fine grains. For $V_{in}$ larger than $V_{th}$, we expect a negligible contribution of the fine grains to the total stress, while the contribution is non-zero when $V_{in}$ gets smaller than $V_{th}$.

Fig.10 Schematic diagram of the compressible fluid model. $V_{in}$ is the volume of the pore defined by the coarse grains only and $V_{th}$ corresponds the the inner volume when fine grains jam (volume enclosed by the purple contour)
To identify the jamming transition from a rational point of view and compute the inner volume corresponding to $V_{th}$, we propose to consider the ratio $\lambda = \frac{\text{Tr}(\sigma_f)}{\text{Tr}(\sigma)}$ corresponding to the fraction of the mean stress supported by the fine grains. Fine grains get jammed as soon as $\lambda$ rises from zero. Considering the obvious jamming case in Figure 7 (size ratio: 10, fine particle number: 600; size ratio: 5, fine particle number: 80), a threshold value $\lambda_{th} = 5\%$ can be proposed as a rational definition for jamming. The condition $\lambda = \lambda_{th}$ enable to define the jamming volume $V_{th}$ and then estimate $K$ matrices for 600, 700 and 800 fine grains with a size ratio of 10 based on Eq. (4). The components of $K$ are displayed in Figure 11. Note that, the off-diagonal elements of the $K$ matrix are equal to 0 because of the boundary conditions (frictionless bounding walls).

![Fig.11 Evolution of $K_{zz}$ and $K_{xx}$ with different fines numbers](image)

Results in Figure 11 suggest that $K$ is not isotropic. With $K_{zz} > K_{xx} = K_{yy}$, which is consistent with the anisotropic microstructure induced by the external loading imposed to the cell. As a result, the compressible fluid model (isotropic compressibility) is not satisfactory, and fine grains contribute to stress anisotropy. However, as shown in Figure 11, $K$ stays constant when fines are activated, which implies that $K_{zz}, K_{xx}$, and $K_{yy}$ can be interpreted as
anisotropic compressibility moduli. It is clear from Figure 12 that the moduli increase as the number of fine grains increases, while the anisotropy stays almost constant with $\frac{K_{zz}}{K_{xx}} = 2^2$.

![Figure 12](image)

**Fig.12** (a) Mean $K_{zz}$ and $K_{xx}$ with different fines numbers (600 to 800); (b) anisotropy $K_{zz}/K_{xx}$ with different fines numbers

While oversimplifying real microstructures, the present approach on idealized mesostructures enables to investigate the qualitative and quantitative effects of fine grains on the average stress tensor in bi-disperse granular materials. The initial assumption that the stress within fine grains can be described by a spherical matrix does not hold and it was shown that fine grains contribute to a limited stress anisotropy with jamming not controlled by the local porosity. In addition, in some cases, the jamming point is observed in the dilatancy regime (a small increase of volume in the H-cell is observed after the jamming point). Consequently, the process of jamming is not necessarily controlled by the volume $V_{th}$ as assumed in Eq. (4).

**Systematic jamming investigation with directional analysis**

The results of 3D numerical simulations show that the stress state of the fine particles cannot be modelled as a compressible fluid model. In order to explore the jamming process of fine grains more deeply and more comprehensively (assess the relative contributions of isotropic and shear jamming

\[2^2\] Note that for an opening angle of 60° in the H-cell, the geometrical aspect ratio $L_1/L_2$ is close to 1.15. As shown later on, the fine stress anisotropy is indeed not controlled by the geometrical anisotropy of the H-cell.
mechanisms), we perform in this section complementary strain controlled directional analyses. For the sake of simplicity and better visualization, the analysis is carried out with the 2D version of the H-model, even though the method can be readily transposed to 3D conditions. To make the computation of the sample porosity and fine content easier\(^3\), the 2D H-cell is filled with fine grains in the whole box space (and not only in the inner space) as illustrated in Figure 13. A 2D fines content of 25% is considered in this section with a size ratio of 10.

**Iso-activation surfaces**

As in the previous section, fine grains jamming is quantified by considering the ratio \( \lambda = \frac{p_{\text{fine}}}{p_{\text{coarse}}} \), where \( p_{\text{fine}} \) and \( p_{\text{coarse}} \) are the mean stress contribution of fine and coarse grains respectively according to Eq. (3).

\[ \delta L_1 \]

\[ \frac{L_1}{\delta L_1} \]

\[ \frac{L_2}{\delta L_2} \]

**Fig.13** Schematic graph of directional analysis in 2D H-cell considering fine content

Before conducting the directional analysis, the H-cell filled with fine grains is first isotropically compressed up to 10 kPa. Then, an incremental variation of the cell dimensions is imposed as

\(^3\) In 3D, no analytical formula exists to compute the inner volume of the H-cell and the inner volume was assessed numerically in the previous section. In addition, the use of the bounding box as the meso-volume is more consistent with the strain localization hypothesis used in the H-model.
\[ \begin{align*}
\frac{\delta L_1}{L_1} &= \delta \varepsilon \sin \theta \\
\frac{\delta L_2}{L_2} &= \delta \varepsilon \cos \theta
\end{align*} \]  \tag{5}

where \( \delta \varepsilon > 0 \) and \( \theta \in [135^\circ, 315^\circ] \).

The strain loading paths are shown in Figure 14 for different loading angles \( \theta \). Isotropic jamming is observed for \( \theta = 225^\circ \), while shear jamming is obtained for \( \theta = 135^\circ \) and \( \theta = 315^\circ \). The parallel dash lines represent iso-variations of the meso-volume \( V_{meso} = L_1 L_2 \), since

\[ \frac{\delta V_{meso}}{V_{meso}} = \frac{\delta L_1}{L_1} + \frac{\delta L_2}{L_2} \]  \tag{6}

Should jamming be controlled by the inner volume of the mesoscale H-cell, iso-activation surfaces (i.e. iso-values of \( \lambda \), 5\% and 10\% for instance) are expected to be parallel to the dash curve. However, iso-activation surfaces have a more complex shape, which demonstrates that fine activation is not only controlled by the change of inner volume of H-cell. Moreover, comparing the shape obtained for \( \lambda = 5\% \) and \( \lambda = 10\% \), it is shown that iso-activation surfaces are not perfectly homothetic (their shapes are not derived from a simple rescaling).
Because the contribution of fine grains to stress stems from the compaction of the fine population (jamming state) leading elastic energy storage at contacts, it is interesting to consider iso-values of the ratio between elastic energy stored in c-c contacts over elastic energy stored in c-f and f-f contacts. For a given class of contacts (c-c only or c-f and f-f), the elastic energy is computed as

\[
E_{pot} = \sum_c \frac{1}{2} \left( \frac{f_n^c}{k_n} + \frac{f_t^c}{k_t} \right)
\]

where \(f_n^c, f_t^c\) are the normal and tangential contact forces at contact \(c\) and \(k_n\) and \(k_t\) the normal and tangential contact stiffness. Therefore, the ratio of potential energy in fine and coarse grains can be defined as \(\lambda_c = \left( E_{pot}^{c-f} + E_{pot}^{f-f} \right) / E_{pot}^{c-c}\), activation surfaces of potential energy (\(\lambda_c = 5\%, 10\%)\) are thus displayed in Figure 15.
According to Figure 15, the activation surface of potential energy is shown as a right-angle triangle with sides parallel to the axis. For example, whatever the loading direction between 150 degrees and 210 degrees, activation surfaces corresponding to $\lambda = 5\%$ or $10\%$ are reached for the same level of deformation in $L_2$ direction. The same phenomenon was observed in the strain intensity of $L_1$ direction when $\theta$ from 240 degrees to 300 degrees. This means that the ratio of the stored elastic energy depends mostly on the largest contraction of the cell dimensions $L_1$ or $L_2$. In other words, the amount of the elastic energy that is stored in the fine grains mostly depends on the principal compression of the H-cell. It should be interesting to assess whether this result holds true in mesostructures at REV scale in DEM simulations. In addition, Figure 15 shows that the activation surfaces are more homothetic for the stored energy than for the mean stress contribution. However, the homothetic coefficient is different from 2 when the $\lambda_e$ is doubled from $5\%$ to $10\%$, which highlights a nonlinear relationship between the fraction of elastic stored energy and the strain intensity (from -0.121 to -0.196 in $L_1$ direction, and from -0.141 to -0.264 in $L_2$ direction as shown in Figure 15).

**Incremental stress responses**
To better understand the contribution of fine grains to the contact stress, the incremental fine grain stress corresponding to incremental strain variations are shown in Figure 16. The purple points connected by the dash line correspond to an incremental strain magnitude \( \delta \varepsilon = \sqrt{\left(\frac{\delta L_1}{L_1}\right)^2 + \left(\frac{\delta L_2}{L_2}\right)^2} = 5\% \).

Fig. 16 (a) Strain directional analysis surface; (b) evolution of stress contribution of fine grains

The evolution of the stress contribution of fine grains (as computed from the c-f and f-f in Eq. (3)) is shown in Figure 16(b). The hollow symbols correspond to strain magnitudes of 1\%, 3\% and 5\%. The stress growth in \( (d\sigma_{xx,\text{fine}}, d\sigma_{zz,\text{fine}}) \) plane is quasi-linear whatever the loading direction. For \( \theta = 225^\circ \), the slope of horizontal and vertical fine stress is close to one, which means that isotropic contraction of the H-cell generates an isotropic compression of the fine grains despite the anisotropy in the coarse grains’ geometry.

To better analyze the results, it is then convenient to set the iso-compression and iso-contraction directions as reference directions. As illustrated in Figure 16 (a) and (b), we define \( \theta_{\text{strain}} \) and \( \theta_{\text{stress}} \) such that the iso-compression direction corresponds to \( \theta_{\text{strain}} = \theta_{\text{stress}} = 0^\circ \). In the directional analysis, \( \theta_{\text{strain}} \) vary from \(-90^\circ\) (constant volume, compression along x
direction) to $+90^\circ$ (constant volume, compression along $z$ direction). The relationship between $\theta_{\text{strain}}$ and $\theta_{\text{stress}}$ is shown in Figure 17.

![Figure 17](image)

**Fig. 17** Relationship between the stress angle $\theta_{\text{stress}}$ and the strain angle $\theta_{\text{strain}}$ for different strain magnitudes. The phenomenological fit proposed in Section 4 is shown (dashed lines).

Figure 17 reveals that $\theta_{\text{stress}}$ decreases with $\theta_{\text{strain}}$ in a step form. For small and large values for $\theta_{\text{strain}}$, $\theta_{\text{stress}}$ is nearly constant with $\theta_{\text{stress}} \in [-20^\circ, 20^\circ]$. This demonstrates that the fine contribution to the contact stress has a limited anisotropy whatever the loading direction. Moreover, the fact that $\theta_{\text{stress}}(\theta_{\text{strain}} \to 90^\circ) = -\theta_{\text{stress}}(\theta_{\text{strain}} \to -90^\circ) \simeq -20^\circ$ shows that the stress anisotropy depends mostly on the contraction direction ($x$ or $z$), independently from the H-cell anisotropy. This result is consistent with the activation surfaces of potential energy shown in Figure 15. Thus, the principal compression direction drives alone the amount of stored energy in the fine grains contacts.

The observed anisotropy in Figure 17 is consistent with the observed anisotropy of the $K$ matrix discussed in second section for the 3D case, where $K_{zz}/K_{xx} = 2$. Since $\frac{K_{zz}}{K_{xx}} = \frac{d\sigma_{zz,\text{fine}}}{d\sigma_{xx,\text{fine}}} = \tan\left(\frac{\pi}{4} - \theta_{\text{stress}}\right)$, such an anisotropy corresponds to $\theta_{\text{stress}} = \frac{\pi}{4} - \arctan(2) = -18^\circ$. 
In addition to the relationship between $\theta_{\text{stress}}$ and $\theta_{\text{strain}}$, the magnitude of the incremental fine stress $\left|d\sigma\right| = \sqrt{d\sigma^2_{xx,\text{fine}} + d\sigma^2_{zz,\text{fine}}}$ is given in Figure 18 as a function of $\theta_{\text{strain}}$ and $\delta \varepsilon$.

![Graph](image)

**Fig.18** Fine stress evolution as a function of $\theta_{\text{strain}}$ and strain magnitude $\delta \varepsilon$. The phenomenological fit proposed in Section 4 is shown (dashed lines).

The stress magnitude shows a slight dependence to the strain loading direction while being symmetrical with respect to $\theta_{\text{strain}} = 0$. The largest increase in the stress magnitude is observed along isotropic compression loading path while pure shear loading paths corresponds to smaller fine stress magnitude. This means that fines turn out to be less stiff in shear jamming than isotropic jamming. This is consistent indeed with the distinction between shear jamming and isotropic jamming that is reported in the literature (Bi et al. 2011; Behringer et al. 2014; Luding 2016). Shear jamming forms for smaller densities but the shear modulus of shear jammed material is usually smaller than the bulk modulus of isotropically jammed materials (Zhao et al. 2011). Not surprisingly, the stress magnitude is strongly influenced by the incremental strain magnitude, exemplifying a nonlinear dependence consistent with the homothetic coefficient in Figure 15 being different from the strain intensity ratio.
Overall, we can summarize the main properties of the fine stress observed in Figures 17 and 18 as follows:

- Isotropic contraction corresponds to isotropic compression: $\theta_{\text{stress}}(\theta_{\text{strain}} = 0^\circ) = 0^\circ$
- As soon as the imposed contraction anisotropy is large enough, the stress response exhibits a constant anisotropy oriented in the principal contraction direction
- The stress intensity grows non-linearly with the strain intensity
- The stress intensity is larger for isotropic contraction and approximately symmetric with respect to the contraction direction $\pm \theta_{\text{strain}}$.

**An analytical model to account for fine grain contribution to stress**

In order to have an efficient implementation of the fine stress in the H-model, there is a need to propose an analytical relationship to describe the contribution of fine grains to the stress. Such a relationship should respect the main properties observed in Figure 17 and 18 and summarized in the end of the previous section.

The general form for the fine stress $d\sigma_f$ can be written as

$$d\sigma_f = \left| d\sigma_f \right| \begin{pmatrix} \cos \left( \frac{\pi}{4} - \theta_{\text{stress}} \right) & 0 \\ 0 & \cos \left( \frac{\pi}{4} + \theta_{\text{stress}} \right) \end{pmatrix}$$

where $\theta_{\text{stress}}$ is defined on Figure 16 (b).

From Figure 17, the relationship between $\theta_{\text{stress}}$ and $\theta_{\text{strain}}$ can be sought as

$$\theta_{\text{stress}} = \theta_0 \arctan(\beta \theta_{\text{strain}})$$

where $\theta_0$ represent the maximum stress anisotropy and $\beta$ the sensitivity to the strain directions for incremental evolutions close to the isotropic compression case. In this study, a satisfying approximation of the data is obtained with $\theta_0 = 13.5^\circ$ and $\beta = -3$. 
As for $\|d\sigma_f\|$, Figure 18 suggests that the stress magnitude can be written as,

$$\|d\sigma_f\| = A\delta\varepsilon^\alpha \cos(\omega\theta_{\text{strain}})$$ \hfill (10)

where $A$ accounts for the bulk fine grains’ stiffness, $\omega$ controls the sensitivity to the strain loading direction and $\alpha$ models the non-linearity with respect to the strain intensity. A reasonable fit is obtained for $\alpha = \frac{3}{2}$, $A = 1.6$ MPa, and $\omega = 0.5$. The fitting function is displayed in Figure 18.

Overall, the anisotropic model for fine contribution to stress can be written as

$$d\sigma_f = A\delta\varepsilon^\alpha \cos(\omega\theta_{\text{strain}}) \begin{pmatrix} \cos(\frac{\pi}{4} - \theta_0 \arctan(\beta\theta_{\text{strain}})) & 0 \\ 0 & \cos(\frac{\pi}{4} + \theta_0 \arctan(\beta\theta_{\text{strain}})) \end{pmatrix}$$ \hfill (11)

with

$$d\varepsilon = \begin{pmatrix} -\frac{\delta L_2}{L_2} & 0 \\ 0 & -\frac{\delta L_1}{L_1} \end{pmatrix} = \delta\varepsilon \begin{pmatrix} \sin(\frac{\pi}{4} - \theta_{\text{strain}}) & 0 \\ 0 & \cos(\frac{\pi}{4} - \theta_{\text{strain}}) \end{pmatrix}$$ \hfill (12)

where $\theta_{\text{strain}} \in [-90^\circ, 90^\circ]$ is defined on Figure 16 (a) and $\delta\varepsilon > 0$. In Eq. (11) and (12), soil mechanics conventions are used with positive compressions and positive contractions. This fit accounts for most of the properties observed in Figures 16 to 18.

As shown in Eq. (11), five parameters are introduced in the model to reflect the effect of fine at mesoscale. To verify whether these parameters can account for the fine stress response in Figure 16(b), the analytical predictions are compared with the DEM results in Figure 19.
As shown in Figure 19, the analytical model account fairly well for the fine grain contribution to the contact stress. The proposed 2D model is thus able to catch the main characteristics of the fine stress behavior.

When moving from 2D to 3D conditions, the number of kinematic degrees of freedom of the system increases dramatically, especially because of the connectivity of the pore space. Even though additionnal work is required to extend the model given in Equation (11) to 3D conditions and varying fine contents and grain aspect ratios, the following results should hold true as far as the mesoscopic cell scale is considered:

- The mean stress contribution of fine grains is neither controlled by the volumetric strain, nor a linear function of the strain magnitude. However, this contribution is the largest one in case of isotropic jamming.

- The anisotropy of the fine contribution to stress is controlled by the maximum compression direction.
- The anisotropy of the fine contribution to stress remains limited, whatever the strain anisotropy considered.

**Conclusion and outlook**

In this study, it has been shown how DEM simulations at mesoscopic scale can be used to investigate the contribution of fine grains to the contact stress. By considering H-cells filled with various fine grains numbers and sizes, the jamming process of the fine grains has been explored along triaxial and incremental proportional loading paths (through strain controlled directional analyses). With use of mesoscale quantities such as contact numbers and stress decomposition, it was shown that fine grains get jammed progressively depending on the fine content and the size ratio. By performing directional analysis, the stress contribution of fine grains was proved not to be always isotropic but to exhibit a limited anisotropy driven by the largest compression direction. Except for loading conditions close to isotropic compression, the stress anisotropy ratio in fine grains is found to be close to 2 for the fine contents and size ratios considered in this study. Derived from the directional analysis, an analytical model with five parameters has been shown to account for the fine grain contribution to the stress. This model, which is more complex than a simplistic compressible fluid activated when the internal volume of the H-cell is smaller than a threshold volume, provides a satisfying fit of the DEM results.

In addition to these general findings, the detailed conclusions from the present study are summarized below.

(1) Small fine contents correspond to well-marked jamming transition characterized by a sharp increase of the fine grain stress and a sharp increase in contact numbers. When the fine content increases, the jamming transition becomes smoother.
(2) For 3D H-cells, we define a matrix $\sigma_f$ to describe the stress contribution of fine grains. By dividing $\sigma_f$ by the cumulated volumetric strain from the jamming point, a compressibility matrix $K$ is built. The results show that $K$ is diagonal but not spherical. $K$ exhibits a transverse isotropy in axisymmetric triaxial loading, which corresponds to the anisotropic microstructure induced by the external loading and not to the H-cell anisotropic geometry. $K$ tensor stays constant along triaxial loading when fines are activated and the anisotropy ratio remains almost constant ($K_{\text{max}}/K_{\text{min}} = 2$) whatever the fines number.

(3) Through the directional analysis of different stress path loading results, we showed that the mean stress contribution of fine grains is not controlled by the volumetric strain and is not a linear function of the strain magnitude. By looking at iso-contributions of fine grains to the elastic energy, it was shown that the maximum contraction in $x$ or $z$ direction mainly controls the jamming process.

(4) DEM enabled to propose a refined model embedding the anisotropic contribution of fine to the mesostress. By fitting the results of directional analysis, a stress-strain relationship of fine grains has been derived, and a mesoscopic constitutive model with five parameters has been proposed. The model was shown to account for the main characteristics of the fine grains’ contribution to the global stress.

In order to confirm the preliminary results derived in this study on the contribution of fine to the stress development within an idealized bi-disperse granular specimen, it will be needed to test different fine contents and coarse/fine sizes ratios. Then, the proposed model will be implemented into the H-model to address larger engineering scales. The enriched version of the H-model with fines will then be tested against laboratory tests at representative elementary volume scale before moving to the structure scale. As a possible application, the enriched H-model accounting for fine grains will be used to explore the influence of fine grains on material instability, with a special focus to the consequences of suffusion, a special form of internal
erosion for which the smallest particles of a soil are eroded by an internal fluid flow. Today, the mechanical consequences of suffusion, and in particular the impact on instability mechanisms is not well accounted for in constitutive models. A multiscale model incorporating the physics of fine grain jamming will be of great interest to better model the failure modes of dams or landslide deposits subjected to internal fluid flows, and better anticipate their catastrophic consequences.

**Data Availability**

The data that support the findings of this study were generated using the DEM code LIGGGHTS. Data are available upon request.

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**References**


