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On definition of a relevant meso-scale for upscaling the mechanical behavior of 3D granular materials

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Abstract In this paper, the difficulty to adapt the definition of a meso-scale for 2D granular materials to derive the macroscopic mechanical behavior of 3D granular materials by upscaling is discussed. A starting point for a definition of a 3D meso-scale may be found in previous works where the transport of small particles through a set of defined pores and constrictions has been investigated. In this framework, different methods to derive a set of pores on which can be defined 3D meso-domains have been compared. Some clues are given about their relevancy to address the macroscopic mechanical behavior of 3D granular materials using an upscaling from a meso-scale.

Keywords 3D granular materials · DEM · Mechanical behavior · Upscaling · Meso-scale · Merging criteria

1 Introduction

The macroscopic mechanical behavior of 2D granular materials has been derived from a meso-scale using an upscaling approach [1–6]. Such a 2D meso-scale can be defined at the level of closed loops composed of pairs of contacting particles. Nguyen *et al.* [3,4] presented a method to construct these closed loops for 2D granular assemblies of disks based on Delaunay triangulation.

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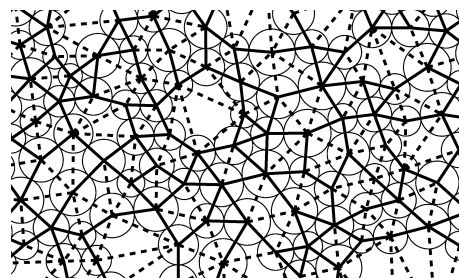


Fig. 1 Part of a 2D granular assembly is subdivided into closed-loops. Solid and dashed lines depict a closed and an open branch, respectively.

First, this method consists in paving the studied domain into triangles, each of which joining the centers of three neighboring particles. In this Delaunay network, a branch is considered as *closed* if it joins two contacting particles or as *open* otherwise as illustrated in Figure 1. Every couple of adjacent triangles that share an open branch are then merged together. In doing so, each set of merged triangles forms a closed loop denoted *meso-domain*.

The local fabric of each meso-domain is described by a loop tensor proposed by Satake *et al.* [1], from which the elongation direction and degree of each meso-domain are derived [3]. The strain and stress tensors associated to each meso-domain are defined from the particle movements and contact forces, respectively [2–4]. Nguyen *et al.* [6] validated afterwards this new upscaling approach to obtain the macroscopic mechanical behavior of 2D granular materials from that of the meso-domains.

Such a meso-scale holds a definite physical meaning since important information such as the topology of the contact network and the arrangement of particles creating the meso-domains is *de facto* taken into account. However, the definition of this meso-scale for 2D materials cannot be straightforwardly extended to the 3D

case since a 3D granular material has a much more complex micro-structure. Indeed, while each meso-domain for a 2D granular material clearly defines a closed pore which is not interconnected to its neighboring pores, the void space in a 3D granular material is characterized by a set of larger voids interconnected by smaller voids also denoted *constrictions*. A question that arises here is whether there exists a relevant meso-scale for 3D granular materials at which the features observed for 2D materials can be recovered. Moreover, are only 3D meso-domains composed of particles in mutual contact suited for a mechanical upscaling? Therefore, the definition of a relevant meso-scale for 3D granular materials seems a challenging and a complex task.

This paper presents some methods to define a 3D meso-scale, which can be envisioned as potential answers to the aforementioned questions. These methods come from another research domain where a partition of the void space of a granular material into pores and constrictions was provided. In particular, it was used to study the phenomena of transport and blockage of flowing smaller particles in a granular filter.

A comparison of the obtained sets of 3D meso-domains by these different methods is provided. This study mainly aims to pave the way to define a meso-scale for 3D granular materials. The validation of a given set of meso-domains as a relevant meso-scale in an upscaling approach for studying the mechanical behavior is beyond the scope of this work.

2 Weighted Delaunay triangulation

The 3D weighted Delaunay triangulation [7] provides a partition of a packing of spheres into tetrahedra whose vertices correspond to the centers of four neighboring particles. In this partition, the weight associated to each sphere is equal to the square of its radius. However, the main drawback of this tessellation technique is that it tends to subdivide single pores into several smaller pores and it results in a uniform pore network for which each pore is systematically associated to four exits (constrictions) located on the four faces of each tetrahedron [9,10]. Therefore, neighboring tetrahedra need to be merged according to a given criterion to obtain an accurate representation of the void space of a granular assembly [9–15]. In the following, we introduce a concept of *sub-domains* which are defined as polyhedral volumes composed of one tetrahedron or several merged tetrahedra. Each sub-domain is a candidate for being a meso-domain once the merging process finishes. Different merging criteria have been proposed and they can be classified into three main categories: (i) criteria based on contacts between particles, (ii) criteria based

on a possible overlapping between the inscribed void spheres of two adjacent tetrahedra, and (iii) criteria based on the porosity of a face and those of the two adjacent sub-domains that share this common face.

3 Criteria based on contacts

By drawing an analogy between the 2D and 3D Delaunay networks, one might translate the concept of closed branches for 2D case to 3D case by considering that a triangular face shared by two adjacent tetrahedra is a closed loop if it connects three neighboring particles in mutual contact. In other words, a triangular face is open if it connects, at least, one couple of particles which are not in contact. Two adjacent tetrahedra that share an open face are then merged together. With such a merging criterion, we found that may be generated a very big meso-domain that occupies more than 70% of the total volume of the sample. Consequently, the merging criterion used for 2D case cannot be straightforwardly extended to 3D case.

O’Sullivan *et al.* [8] relaxed the above concept of closed loops for 3D materials. According to this method, a 3D closed loop is composed of either one triangular face with three contacts or two adjacent triangular faces with four contacts. Two adjacent pores must share a closed loop, otherwise they are merged together. This concept is appealing; however, the feasibility to define the meso-domains needs to be further investigated. This method is not studied here and the reader can refer to [8] for more details.

Instead of requiring that the particles of a meso-domain must form closed loops of three or four contacts, we require in the following merging criteria that the particles of a meso-domain are sufficiently close to each other, *i.e.* the space between them is sufficiently small, so that they can form an appropriate arrangement to resist shear loading.

4 Criteria based on overlapping inscribed void spheres

These criteria first consist in defining an inscribed void sphere for each tetrahedron and then in merging adjacent tetrahedra depending on the possible overlapping between their inscribed void spheres. Some criteria merge every two adjacent tetrahedra if there exists an overlapping between their inscribed void spheres [10,12,14]. Other relaxed criteria make use of a threshold value directly related to the intensity of overlapping [9,13]. For instance, Al-Raoush *et al.* [9] proposed to merge two adjacent tetrahedra if the center of one of the two

associated inscribed void sphere is located within the other one.

Reboul *et al.* [10] adopted a strict criterion to merge tetrahedra in the primary partition given by the weighted Delaunay triangulation (called L_0). To avoid over-merging of tetrahedra, the authors introduced a merging level L_1 , for which only the tetrahedron with the largest inscribed void sphere and its direct neighbors are merged at each merging step. Seblany *et al.* [14] subsequently modified this merging criterion by introducing a merging level L'_0 to eliminate **strongly flat tetrahedra issued from the weighted Delaunay triangulation**. This level consists in merging every couple of adjacent tetrahedra if the overlapping of the corresponding inscribed void spheres is greater than 99.9999% or if the constriction size is greater than the size of the corresponding inscribed void spheres. By doing so, about 10% of the couples of adjacent tetrahedra are merged whatever the studied packing of spheres (coefficient of uniformity ranging between 1.5 and 6) and density state (loosest or densest state).

The merging criterion L_1 implies that a maximum of five tetrahedra can be merged to form a single meso-domain. It was found that about 50% and 60% of the meso-domains in respective loose and dense assemblies of spheres having a coefficient of uniformity ranging between 1.5 and 6 are represented by a single tetrahedron [10, 14]. It was also proposed to extent this merging to the neighbors of the adjacent tetrahedra (L_2 criterion) but this criterion did not bring a much more complex set of pores [10, 14].

5 Criteria based on porosities of local particle arrangements

In this approach, a sub-domain is a polyhedral volume composed of one tetrahedron or several adjacent tetrahedra. For each sub-domain, the void space is approximated by an inscribed void sphere. The inscribed void sphere must not intersect adjacent solid particles and its center must be located inside the sub-domain. Starting from the weighted Delaunay triangulation, we proceed iteratively to identify all the sub-domains which do not fulfill this physical requirement and then merge them to their neighbors to form new sub-domains. Thus, this procedure is different from those used by Reboul *et al.* and Seblany *et al.* to define their primary set of sub-domains (respectively L_0 and L'_0 levels). It allows us to eliminate efficiently strongly flat tetrahedra issued from the Delaunay triangulation. After this primary merging procedure (PM), further merging is processed by using the two following criteria based on the facial and spacial porosities [11].

5.1 Merging criterion based on the facial porosity

Two adjacent sub-domains share a face which can be composed of one or several triangular faces. The porosity n_f of a face is defined as $n_f = A_v/A$ where A_v and A are the total void area and the total area of the face. We consider that a face shared by a couple of adjacent sub-domains is open if its porosity n_f is bigger than a threshold value n_f^{th} . Every two adjacent sub-domains which share an open face are merged together. A similar merging criterion was used by Van der Linden *et al.* [15].

5.2 Merging criterion based on the relative facial porosity

The above criterion to define if a face shared by two adjacent sub-domains is open or closed might be relative: it might be considered to be closed if it is shared by two very porous sub-domains but it might be open if it is shared by two compact sub-domains. In this regard, we define a relative facial porosity \hat{n}_f as $\hat{n}_f = n_f / \min(n_1, n_2)$ where n_1 and n_2 are the porosities of the two adjacent sub-domains. A face is considered to be open if the relative facial porosity is bigger than a threshold value \hat{n}_f^{th} .

6 Comparison between different criteria

The different merging techniques presented above are used to partition the loose numerical sample **composed of 2500 spherical particles** that was simulated with the Discrete Element Method and presented by Seblany *et al.* [14]. **This sample with periodic boundary conditions has a porosity of 0.38** and a narrowly graded grain size distribution. The criteria based on the absolute and relative facial porosities, respectively abbreviated as FP and RFP, are used after the primary merging procedure (abbreviated as PM) as described in Section 5. These criteria are compared to the L_1 criterion based on overlapping inscribed void spheres (Section 4). The pore size of each sub-domain is characterized by the diameter of an equivalent void sphere whose volume is equal to the void volume of the sub-domain under consideration. Figures 2 and 3 show this comparison **where different threshold values are used** for the FP and RFP criteria. In both figures, the pore size distribution of the tetrahedra obtained from the weighted Delaunay triangulation is represented by the curve L_0 . It can be seen in Figure 2 that the pore size distribution after the primary merging procedure (in Figure 2, the PM

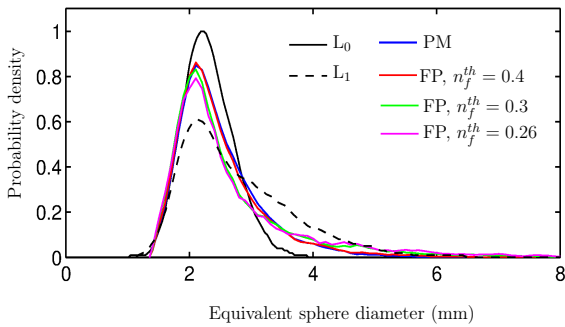


Fig. 2 Probability density versus the equivalent sphere diameter obtained with the L_0 , L_1 , PM and FP criteria.

curve is almost coincident with the red curve) is significantly lowered with larger pore sizes, compared to the L_0 curve. This means that the PM criterion merges efficiently the flat tetrahedra, which have medium or large pore volumes, giving rise to sub-domains with bigger pore volumes. The FP criterion with a threshold value $n_f^{th} = 0.4$ does not notably change the pore size distribution. This means that the PM criterion allows us to eliminate almost highly porous faces ($n_f > 0.4$). A notable change in the pore size distribution can be observed for $n_f^{th} = 0.3$ that leads to some meso-domains with more than 20 tetrahedra. Van der Linden *et al.* [15] recommended a threshold value $n_f^{th} > 0.3$ since a lower threshold value tends to over-merge tetrahedra. We can also remark that the pore size distribution given by the FP criterion with $n_f^{th} = 0.3$ is far from that obtained with the L_1 criterion. This is due to the fact that only 14% of the faces meet the FP criterion with $n_f^{th} = 0.3$, much lower than 30% of the faces that meet the L_1 criterion. One can note that even though the threshold value $n_f^{th} = 0.26$ is chosen such that the number of open faces according to the FP criterion is equal to that given by the L_1 criterion, these criteria give different results. Finally, the FP criterion slightly tends to merge more sub-domains with medium or big void volumes to form new sub-domains with bigger void volumes than the L_1 criterion, while the sub-domains obtained with the L_1 criterion are limited in size. In addition, the sub-domains with low porosities are not affected by the FP criterion as they share most likely faces with low porosities.

Figure 3 shows that the RFP criterion with a threshold value $\hat{n}_f^{th} = 1.0$ does not result in a significant change in the pore size distribution compared to the PM curve. This means that almost all sub-domains obtained after the primary merging technique are less porous than their faces. As the threshold value \hat{n}_f^{th} is reduced, the pore size distribution changes greatly and gets closer to the one obtained with the L_1 criterion. For $\hat{n}_f^{th} = 0.75$, the pore size distribution curve is quite

close to the L_1 curve. We found that about 24% of the faces meet the RFP criterion with $\hat{n}_f^{th} = 0.75$, which is quite close to the number of 30% given by the L_1 criterion, but this is not the only reason to explain the observed result. We have shown previously that, with almost the same number of open faces, the FP criterion with $n_f^{th} = 0.26$ gives quite a different result from that given by the L_1 criterion. Among the closed faces defined by the FP criterion, some of them might be open according to the RFP criterion as they might be shared by adjacent sub-domains of low porosities (their relative porosity becomes bigger than the absolute one) or *vice versa*. Indeed, 6% of the closed faces defined by the FP criterion with $n_f^{th} = 0.26$ become open according to the RFP criterion with $\hat{n}_f^{th} = 0.75$. On the other hand, 24% of the open faces defined by the former become closed according to the latter as they are shared by two sub-domains with high porosities. As a consequence, the RFP criterion merges more sub-domains with small void volumes but less sub-domains with medium or big void volumes than the FP criterion. Finally, in the context of the L_1 merging criterion, it was noted that the overlapping of inscribed void spheres is intrinsically very important in packing of spheres. It means that if two adjacent inscribed void spheres overlap, the opening size of the involved constriction is rather large compared to the pore size of the two corresponding adjacent tetrahedra, leading generally to a high value of the relative porosity \hat{n}_f . It may explain why the RFP criterion with $\hat{n}_f^{th} = 0.75$ gives a pore size distribution close to that given by the L_1 criterion. By comparing Figures 2 and 3, it can be concluded that the RFP criterion provides a better partition of a granular volume into meso-domains than the FP criterion.

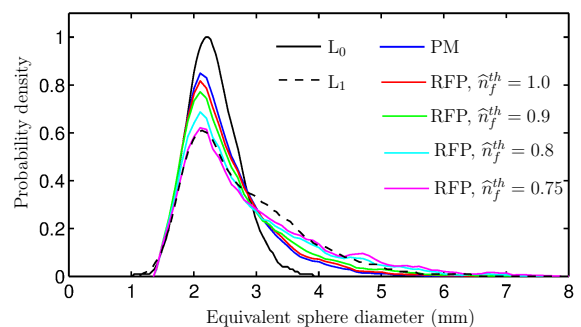


Fig. 3 Probability density versus the equivalent sphere diameter obtained with the L_0 , L_1 , PM and RFP criteria.

7 Discussion

The L_1 and RFP criteria provide a complete partition of a given 3D granular material into meso-domains. In particular, strongly flat tetrahedra that do not hold any

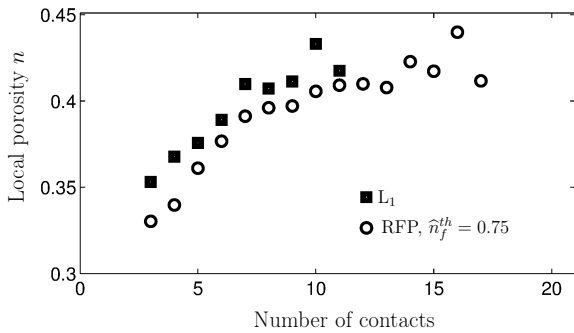


Fig. 4 Correlation between the local porosity and the number of contacts for the meso-domains obtained with the L_1 and RFP criteria with $\hat{n}_f^{th} = 0.75$.

physical meaning are removed from the weighted Delaunay triangulation by using the L'_0 level in the L_1 criterion or the primary merging procedure in the RFP criterion. Both criteria give the meso-domains of different sizes and shapes, which may reflect the inherent heterogeneity of the internal state of granular materials.

Figure 4 shows that the local porosity of the meso-domains obtained with the L_1 and RFP criteria versus their number of contacts. In this figure, a mean porosity is calculated over all the meso-domains having the same number of contacts. This figure shows that there is a strong correlation between the local porosity and the number of contacts within the meso-domains for both criteria: meso-domains with higher number of contacts tend to occupy zones with higher porosity. This correlation was also observed for 2D closed loops [3]. This preliminary result suggests that although both criteria are based on the void space between neighboring particles, mechanical properties of the meso-domains related to contacts between particles (those observed for 2D closed loops) might be recovered for 3D materials.

For these reasons, the meso-domains defined by either the L_1 or RFP criterion hold some basic features for being a possible candidate to develop an upscaling approach for the mechanical behavior of 3D granular materials.

8 Conclusion

In this paper, we proposed two methods to extend the concept of a meso-scale defined initially for 2D granular materials to 3D media. These methods are based on the weighted Delaunay triangulation where adjacent tetrahedra are merged by using criteria holding a physical meaning. Two specific criteria, which take into consideration the void space within local arrangements of particles, were investigated. It was shown that both led to similar partitions of the space into a set of meso-

domains. They hold some basic features to be possible candidates for defining a meso-scale on which a mechanical upscaling of a 3D granular material can be applied. Further evidence must be given in this respect and a deeper study will be carried in a future paper.

Compliance with ethical standards

Conflict of Interest: The authors declare that they have no conflict of interest

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