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Rapid Note

Comparison of two representations of a random cut of identical sphere packing

L. Oger[1,a], P. Richard[1], J.P. Troadec[1], and A. Gervois[2]

[1] Groupe Matière Condensée et Matériaux[b], Université de Rennes 1, 35042 Rennes Cedex, France
[2] Service de Physique Théorique, DSM, CEA/Saclay, 91191 Gif-sur-Yvette Cedex, France

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Abstract. We compare two-dimensional froths obtained by radical tessellation of random planar cuts made through disordered assemblies of monosize spheres at different packing fractions C from $C = 0$ to $C = 0.64$ with two-dimensional stereological cuts obtained through the three-dimensional froths made with the same packing. We have built numerically the packings using different algorithms. The study of both topological and metric properties shows significant differences between the two representations.

PACS. 61.43.Bn Structural modeling: serial-addition models, computer simulation – 61.20.Ja Computer simulation of liquid structure

1 Introduction

In the last decade, scientists have not studied intensively the geometry of real granular media. Except for some global quantities like packing fraction [1,2], the study of such media is difficult. Only indirect measurements using stereological methods on packings of spheres [3–5] have been performed previously. A more detailed investigation is possible when modeling granular media by numerical packings of spheres. In that context, a new approach, based on Voronoï or radical analysis was first tested on 2D monosized and polydispersed disk packings [6–8]. Recent papers [9–12] have shown that it is also a good tool to study the structural properties of sphere assemblies. We recall that one can associate a froth to any packing of spheres by Voronoï or radical tessellation [13] and that one can best study the properties of the packing in the froth.

The aim of this paper is to compare the topological and metric properties between the 2D stereological cut of the 3D Voronoï tessellation of a packing of identical spheres and the radical tessellation of a 2D cut of the same packing. Because of the existence of different disk sizes in the cut, which provide different kinds of cells, we expect many differences. This study must also be compared with studies performed on 2D random disk assemblies, both numerically generated [7] and actual [6,8].

In Section 2, we define the two kinds of tessellations used in this paper. We describe also the classical stereological parameters which relate a 2D analysis to the 3D real structure. Then, we present in Section 3 the topological (face number distribution, average number of neighbors, and first neighbor correlations) and metric (cell average perimeter and area) characteristics of the cellular tessellations.

2 Voronoï tessellation and stereological background

2.1 Tessellation

Finney has generalized the Voronoï tessellation (for example [14]) in monosize packings of spheres (or disks) [15]. Tessellation consists in building cells surrounding each sphere and analyzing the statistical and topological properties of the cells instead of the geometry of the assemblies of spheres.

The plane bisecting the line segment joining the centers of two equal spherical grains limits their influence zone, and the Voronoï cell of a grain is the smallest convex polyhedron made with all the bisecting planes. This cell completely contains the grain and this grain only. Two grains are (first) neighbors if their cells have one common face. It is possible to build a complete hierarchy of neighbors at any packing fraction without ambiguity. The Voronoï tessellation fills space completely.

[a] e-mail: luc.oger@univ-rennes1.fr
[b] UMR CNRS 6626

The simplest extension of this tessellation for polydisperse assemblies is the radical tessellation [16], the bisecting plane being replaced by the radical plane (all the points in the radical plane have the same tangency length or power for the two spheres). The definition may seem somewhat artificial, but many topological features of the Voronoï tessellation are maintained. With this tessellation, large grains have larger cells than smaller ones, a way of estimating their relative hindrance.

2.2 Basic knowledge on stereological properties

Stereological methods mainly consist in performing planar (2D) or linear (1D) random sections (or cuts) in assemblies of bodies. Provided the assembly is large enough (or if several cuts are performed), the average quantities measured in the cuts may give statistical information on the 3D assembly. In 1953, Smith and Guttmann listed from previous works some general stereological laws [17]. For instance, the cut of a disordered 3D packing gives a 2D assembly of objects with the same packing fraction as that of 3D packing. Furthermore, simple measurements on a random cut give the specific surface area of the solid phase in contact with the porous space. Another quantity of interest is the mean average tangent diameter $\langle H \rangle$ which is proportional to the probability of sectioning a given convex body and is related to its mean curvature [18]. For a sphere, $\langle H \rangle$ is the ordinary diameter D, whereas in the case of polyhedra it can be explicitly calculated from dihedral angles [19,20].

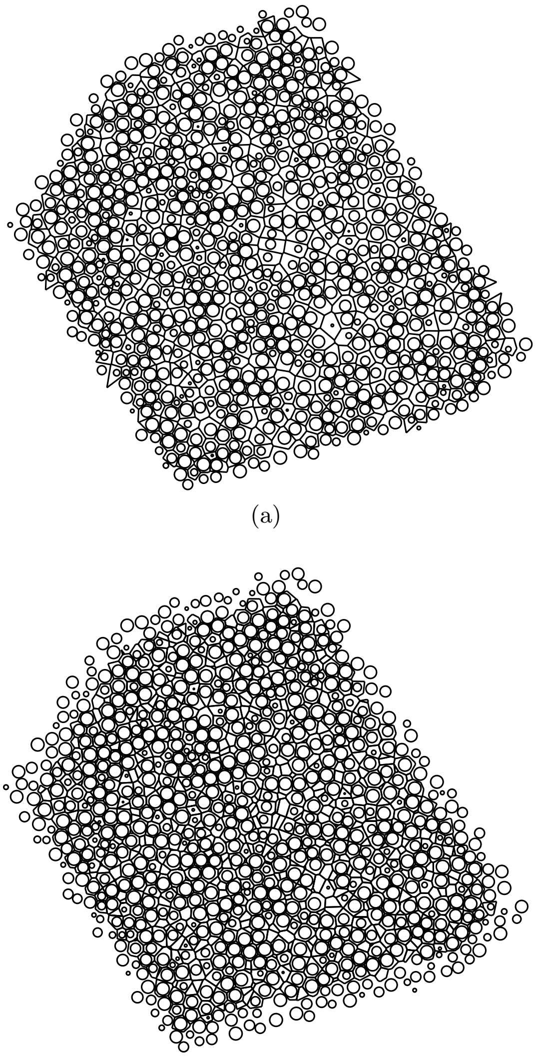
In the case of spherical particles, Weibel [18] and Underwood [21] developed extensions that give some information on the size distribution of the intersection of the spheres with a planar cut. For instance the probability distribution (δ_a) of the diameter d of the disk obtained through a random planar cut of a monosize sphere packing of diameter D is

$$\delta_a(d) = \frac{d}{D\sqrt{D^2 - d^2}} \quad \text{for} \quad 0 \leq d \leq D. \qquad (1)$$

So the mean and variance of the diameters of the section disks are $d_a = \pi D/4$ and $\sigma_a^2 = (32 - 3\pi^2)D^2/48$, which means that many disks of the cut have a diameter around d_a ($\approx 0.78D$). In fact 66% of the disk diameters are larger than $0.75D$.

2.3 Cut tessellations

We have used different algorithms to build disordered monosize sphere packings (collective reorganization, random deposition) with packing fractions varying from 0 up to 0.64 [22]. We have previously studied intensively the topological and metric properties of these packings [9,12,23]. These studies deal with classical Voronoï tessellation using bisecting planes between two spheres. From a 3D structure, we can perform random planar sections through this froth and check conservation of the packing fraction and stereological relation (1).



(a)

(b)

Fig. 1. Representation of the different Voronoï tessellations: (a) radical tessellation of the 2D disk assemblies obtained from the cut of the 3D sphere packing with 650 disks (*2D froth*); (b) 2D planar cut of the polyhedra obtained with the classical Voronoï tessellation of the 3D sphere packing with 985 polygons (*2D cut*).

Two tessellations are considered:

1) a 2D cut of the 3D Voronoï polyhedral froth which represents a peculiar 2D radical froth [24,25] composed of a series of adjacent polygons (the *2D cut*);
2) the 2D radical tessellation of the disks (of various radii) which are the cut of the spheres of the packing (the *2D froth*).

Two neighboring spheres may survive as neighboring disks in the cut. In that case, their radical axis is the intersection of the Voronoï plane with the cut. Thus several edges (and polygons) are identical in the two tessellations. However, some spheres are not intersected by the section plane. They correspond to cells without a circle in their midst in the 2D cut (Fig. 1). Thus, there are some differences in the two tessellations, which are emphasized if the packing fraction decreases. We will now discuss these differences.

3 Results

We obtain results from a series of ten random sections through disordered packings made of 16000 spheres so the statistical study of the 2D tessellations is carried out on about 8000 disks or polygons. Figure 1 presents an example of the two tessellations obtained for the *same cut plane*, on an assembly with packing fraction $C = 0.4$. The *2D froth* is made with 650 intersected spheres (a) and the *2D cut* with 985 polygons obtained by the intersection of the 985 polyhedra with the plane (b). We can see empty cells in the second case. Measurements on ten random sections of the packing of Figure 1 show that the percentage of unoccupied cells is equal to 34%; this is in agreement with the estimated ratio $D/\langle H\rangle$ where $\langle H\rangle$ is calculated assuming that cells are on average not too far from regular polyhedra. The presence of empty cells in the *2D cut* generates a larger distribution of sides n of the cells because some of them, resulting from the section of a polyhedron in the vicinity of a vertex, have few sides. This is true for any packing fraction.

3.1 Topological measurements

The widening of the cell size distribution for the *2D cut* can be seen more precisely in Figure 2a. The two tessellations verify the basic 2D topological law which gives a mean number of sides $\langle n\rangle$ of a 2D tessellation equal to 6, but the dispersion $\mu_2 = \langle n^2\rangle - \langle n\rangle^2$ is very different (2.3 for the *2D cut* and 0.8 for the *2D froth*).

In random 2D froths, the average number of sides $m(n)$ of the first neighbors of a cell with n edges is well fitted by the Aboav-Weaire's law [26,27]:

$$m(n) = \langle n\rangle - a + \frac{\langle n\rangle a + \mu_2}{n}, \qquad (2)$$

where a is a parameter that depends on the froth and $\langle n\rangle = 6$. Figure 2b shows that this law is also rather well obeyed in the two tessellations. Indeed, the variation of $n\, m(n)$ *versus* n is linear; only the slopes are different- for all analyzed packing fractions: the slope of the *2D cut* is 5.4 ± 0.1 while that of the *2D froth* is 4.7 ± 0.1. For comparison, we have made the same measurements on random 2D assemblies of disks with the same packing fractions and the same size distributions as that for the disks of the *2D froth* (obtained from Eq. (1)). The two distributions $p(n)$ are close to one another as shown in Figure 2a, and the variations of $n\ m(n)$ *versus* n are practically the same. This result confirms the randomness of the disk assemblies obtained from our three-dimensional packing.

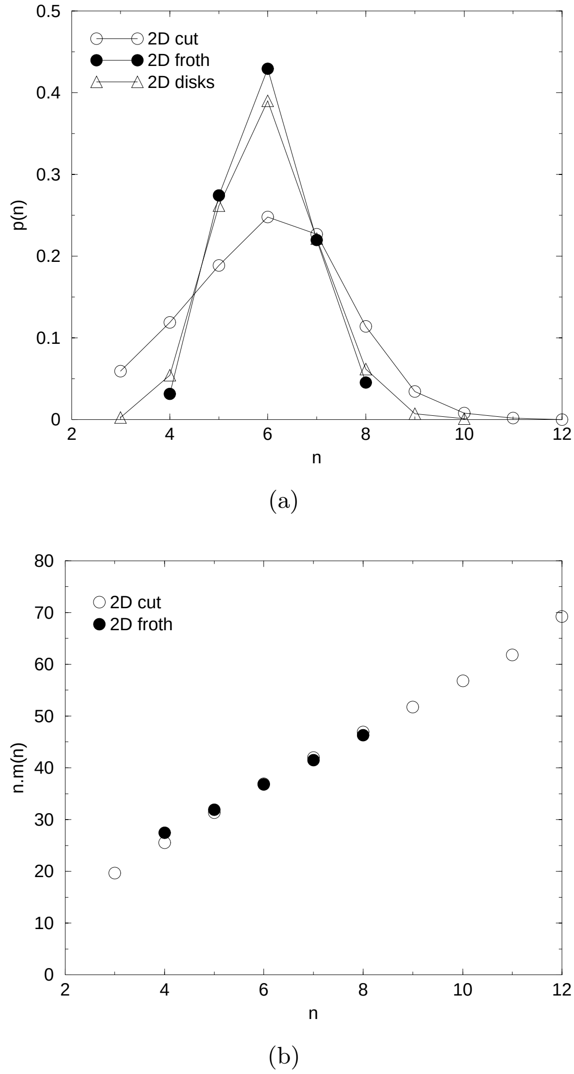
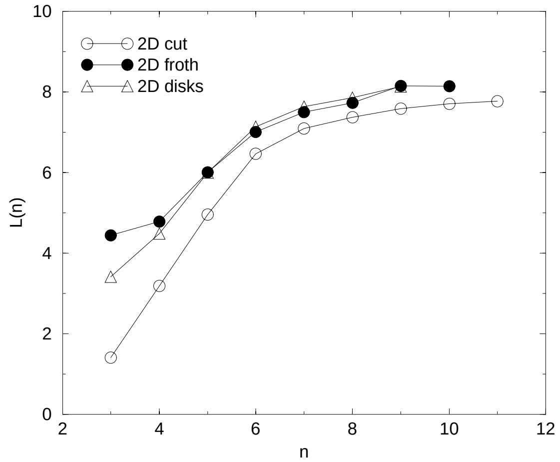


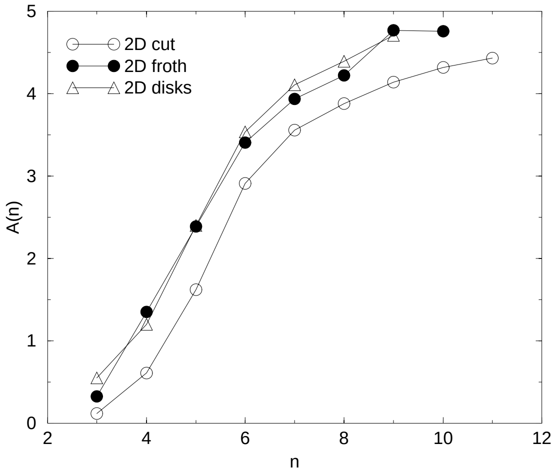
Fig. 2. Topological measurements: (a) distribution of the number of sides of the cell assemblies with a packing fraction $C = 0.4$ of the three kinds of tessellations; (b) Aboav-Weaire's law for the*2D cut* and *2D froth* tessellations.

3.2 Metric measurements

Lewis' law and Desch's law respectively predict linear variations for the average area $A(n)$ and the perimeter $L(n)$ of the cells *versus* their number of sides n. As illustrated in Figure 3, these laws do not hold in either the *2D froths*, or the *2D cuts*. The non-linearity is less strong, but is still evident, in more dilute packings (as long as $C > 0.4$), because at a high packing fraction, the size of a polygon depends strongly on the size of the disk inside it. So the variations of $A(n)$ and $L(n)$ with n depend on the size distribution of the disks, as noted by Annic *et al.* [7]. Again, we have verified that the variations of $A(n)$ and $L(n)$ for



(a)



(b)

Fig. 3. Metric measurements (in radius unity) of the three kinds of tessellation. (a) Distribution of the perimeters of the cell *versus* the number of sides of the cell assemblies with a packing fraction $C = 0.64$. (b) Distribution of the areas of the cell *versus* the number of sides of the cell assemblies with a packing fraction $C = 0.64$.

2D froths are close to that for random assemblies of disks with the same distribution (Fig. 3).

4 Conclusion

The comparison between the two-dimensional froths (*2D froth*) obtained by radical tessellation of random planar cuts made through disordered assemblies of monosize spheres and the 2D stereological cuts (*2D cut*) obtained through the three-dimensional froths made with the same packing gives interesting results. Some properties are valid in the two cases (especially Aboav-Weaire's law) but others differ greatly (metric properties, distribution of sides of polygons). The next two steps will be, first to correlate two-dimensional and three-dimensional properties, and second to extend our analysis to ordered structures or slightly perturbed crystalline structures for which we have previously studied the 3D Voronoï tessellation [28]. We have done some preliminary studies for this point but many random cuts are needed to obtain good statistics. Another approach is the analysis of the disappearance of the empty cells from the *2D cut* in order to obtain the *2D froth* by a series of topological transformations.

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