Modeling of Spherical Particle Packing Structures Using Mathematical Tessellation

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Abstract: In recent years, the literature shows an increasing interest to tessellation methods based on Voronoi diagrams to model different structures as packing of spheres. Voronoi diagrams have found numerous practical and theoretical applications in a large number of fields in science and technology as well as in computer graphics. A useful property of Voronoi diagrams is that they represent cellular structures found in the nature and technology in a natural manner, easily to understand and to design. Although this approach is really not new, meanwhile its intensive use and, consecutively, a systematical study started around 2000 with advances in nanoscience and nanotechnology. In this chapter, two basic tessellation methods are considered in more detail: the Voronoi-Delaunay tessellation and the Voronoi diagram in Laguerre geometry, as well as some of their generalizations. The principal concepts of both tessellation methods are briefly explained for a better understanding of this approach. A review of the related literature is given, focusing mainly on new mathematical tools and several particularities of the applications considered.

Keywords: tessellation, Voronoi diagram, Delaunay simplex, Laguerre geometry, sphere packing, structure modeling.

MSC: 05B45, 05B40, 52B05

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1 Introduction

Tessellation is a relatively new approach for modeling packings of spherical particles. It is based on Voronoi diagrams, which were defined and generalized by G. F. Voronoi in 1908, meanwhile their history traces back to the middle of the nineteenth century by the ideas of Gauss (1840) and Dirichlet (1850) (Aurenhammer, 1991), (Bagi, 2006). An ordinary planar Voronoi diagram can be defined as follows: Given a finite set of distinct, isolated sites in the plane; all locations are associated with the closest one. The result of this assignment is a partitioning of the plane into a set of regions, or polygons, which covers that plane without any gap, and every point of the space belongs to exactly one region (polygon), except those points belonging to the common faces of neighboring regions. The 3D generalization of Voronoi diagrams is widely used for a representation of sphere packings. These diagrams can also be generalized to higher dimensions.

An ordinary tessellation is frequently interpreted as a postal service problem: Given a set of post offices (which represent the sites), where customers want to post their letters, it is necessary to divide the total area into regions for each office, where the people live who obtain their service from the closest office (see, e.g. de Berg et al., 2008). The net of polygons formed by such a division represents a Voronoi diagram for a given set of sites.

In the 3D Euclidian space, a site can be interpreted as an atom or a particle. Then the Voronoi region (polyhedron) for that atom is the volume of the space including all points which are closer to a given atom than to any other atom of the ensemble. The Voronoi diagram of such an atomic system is a network of edges and vertices formed by the edges and vertices of the Voronoi polyhedron.

A didactic interpretation for the visualization of a Voronoi diagram is given by Aurenhammer (1991) through the growth of the crystals in the nature: From several sites fixed in the 3D space, a manifold of crystals starts growing at the same rate in all directions without pushing apart but stopping their growth as soon as they come into contact. The crystal emerging from each site in this process is the region of the space closer to that site than to all others. Icke and van de Weygaert (1991) noted that a Voronoi construction gives not only an insight into the distribution of galaxies in large scales, but it also permits a new approach to the dynamics that mould the shape of the universe we live in. An impressive application of the tessellation approach in architecture was recently presented in the paper by Pottmann et al. (2015).

The actual literature shows an increasing interest to the tessellation methods. The reason is that a tessellation based on a Voronoi diagram contains complete information about the structure of a computer model (Medvedev, 2002). This approach is useful in a large number of versatile fields in science and technology for modeling and describing various natural patterns and for generating random lattices, e.g., for the description and interpolation of a

space in astronomy and geodesy, the study of molecular dynamics and the design of material structures in physics and chemistry, the study of the packing problem in computer sciences, as well as in computer graphics.

The Voronoi diagram is one of the most interesting and useful subjects in computational geometry. Given the visual simplicity and widespread applicability, these concepts were described, interpreted and generalized by various authors due to the diversity of polygonal objects and distance functions. An in-depth up-to-date survey of Voronoi diagrams as a fundamental geometrical data structure was given by Aurenhammer (1991). The author indicated three main reasons for the interest of the researchers in this subject, which is an easily defined and visualized construct: 1) Voronoi diagrams arise in nature in various situations; several natural processes can be used to define particular classes of Voronoi diagrams. Human intuition is often guided by visual perception. If one sees an underlying structure, the whole situation may be understood at a higher level; 2) Voronoi diagrams have interesting and surprising mathematical properties because they are related to many well-known geometrical structures. This has led several authors to believe that the Voronoi diagram is one of the most fundamental constructs defined by a discrete set of points; 3) Voronoi diagrams have proved to be a powerful tool in solving seemingly unrelated computational problems and therefore, they have increasingly attracted the attention of computer scientists in the last few years. Efficient and reasonably simple techniques have been developed for the computer construction and representation of Voronoi diagrams.

Aurenhammer also noted that Voronoi diagrams are useful in the subsequent three respects representing:

- a structure per se that describes explicitly natural processes;
- an auxiliary structure for investigating and calculating related mathematical objects;
- a data structure for algorithmic problems that are inherently geometric ones.

May be a more claimed today's application of Voronoi diagrams is due to pattern recognition of atomic environments and the investigation of the structures of simulated materials. Since the seminal works by Bernal and Finney (1967) and Finney (1970), the tessellation methods based on Voronoi diagrams resulted in a useful computational approach for a geometrical modeling and a statistical study of the structures of the lattices generated by randomly packed spheres for such materials as gases, liquids, glasses, polymers, bones, and others, resolving problems of the modern material science. The revision of the up-to-day literature shows that tessellation techniques are actually the most powerful and perspective approach for

- modeling and simulating ensembles composed of spherical particles,
- the prediction of the metric and topological properties of the packing structures, and
- their statistical analysis.

This chapter deals with principal tessellation methods based on Voronoi diagrams applied to the modeling and analysis of structures described as randomly packed spheres, focusing mainly on the mathematical details and the particularities of the respective application area. A short description of the concepts used is given in Sections 2 and 3. Some important properties of sphere packings, related to the subject of the chapter, are pointed in Section 4. In Sections 5 and 6, the tessellation approaches employed for mono-sized and multi-disperse packings, respectively, are reviewed. Some concluding remarks finish the chapter.

2 Basic properties of the Voronoi-Delaunay tessellation

A generic definition of Voronoi diagrams was given first by Aurenhammer (1991). Let S denote a set of n *sites* or *generator points* in the plane. For two distinct sites $p, q \in S$, the dominance of p over q is defined as the portion of the plane being at least as close to p as to q:

$$\mathrm{dom}(p, q) = \{x \in \boldsymbol{R}^2 | \delta(x, p) \leq \delta(x, q)\},$$

where δ denotes the Euclidean distance function and dom(p,q) is a closed half-plane bounded by the perpendicular bisector of p and q, which separates all points of the plane into two half-planes, closer to p from those closer to q (Figure 1). The region of a site $p \in S$ is the portion of the plane lying in all of the dominances of p over the remaining sites in S:

$$\mathrm{reg}(p) = \cap_{q \in S-\{p\}} \mathrm{dom}\,(p,q).$$

Thus, the regions are created by the intersection of n-1 half-planes. As a consequence, a polygonal partition called the *Voronoi diagram* $V(S)$ or *Dirichlet tessellation*[1] for the finite site-set S is formed. A region reg(p), called the *Voronoi region*, cannot be empty since $p \in$ reg(p) as well as all points of the plane are at least as close to p as to any other sites in S. Such a partition contains exactly n regions, some of them are necessarily unbounded. A *Voronoi edge* is the intersection of two neighboring Voronoi regions, and a *Voronoi vertex* is the intersection of three or more Voronoi regions that share a vertex (Figure 2). Each point on an edge is equidistant from exactly two sites, and each vertex is equidistant from at least three sites. The boundary of a region consists of at most $n - 1$ edges and vertices (their endpoints). If the centers are chosen randomly, a so-called Poisson–Voronoi construction results. An example of a Voronoi diagram is given in Figure 3.

This construction can be easily extended to 3D with planes as bisectors instead of lines. The number of regions, also called faces f_i, of the obtained polyhedron containing the ith particle is its *geometric coordination number*.

[1] For details of the difference between the Voronoi diagram and the Dirichlet tessellation, the reader can consult Bagi (2006)

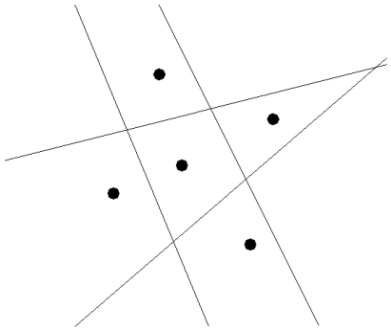


Figure 1. Plane separation mode in a Voronoi diagram.

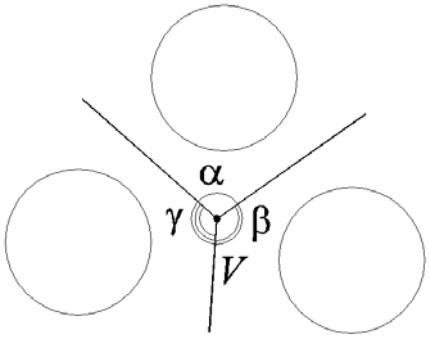


Figure 2. A Voronoi vertex *V* formed by the boundaries with the corners α, β, and γ.

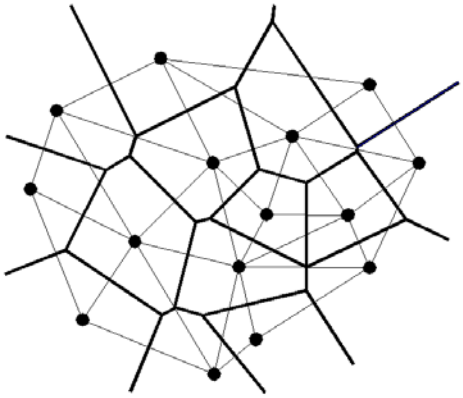


Figure 3. A representation of an ordinary Voronoi diagram for a given set of sites in the plane and the corresponding Delaunay tessellation.

Connecting two sites in the plane by a straight-line edge if and only if their Voronoi regions share a common edge, the Delaunay structure composed of triangles is obtained. The set of edges of these triangles gives the Delaunay tessellation of the set of sites, also referred to as Delaunay triangulation (see Figure 3). The Delaunay triangulation possesses the property that no site falls into the interior of the circumcircle of any triangle in the triangulation. In other words, the circumcircle of the Delaunay triangle is an *empty circle* only if the triangulation of *S* is a Delaunay triangulation.

In the general case, a Delaunay construction decomposes the Euclidean space of dimension *d*, containing a given set of points, into non-overlapping space-filling convex hulls called *Delaunay simplices*, which have not necessarily the same shape and size. A simplex is a point itself, a straight line segment connecting two points, a triangle, or a tetrahedron, called the *zeroth-order simplex*, the *first-order simplex*, the *second-order simplex*, the *third-order simplex*, respectively, and so forth, for $d = 0,1,2,3,\ldots$) (Figure 4).

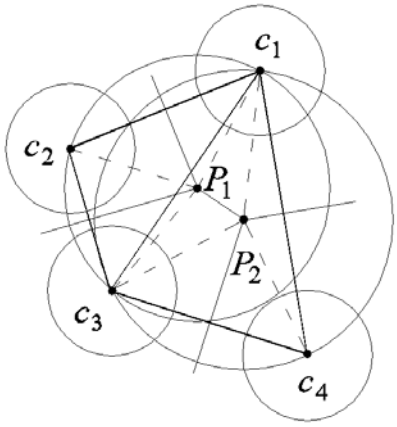


Figure 4. A Delaunay tessellation forming two simplices, and the Voronoi diagram for the circles c_1, c_2, c_3 and c_4. Two Delaunay empty circles with the centers in the points P_1 and P_2; P_1 is equidistant from the centers of the circles c_1, c_2, and c_3 while P_2 is equidistant from the centers of the circles c_1, c_3 and c_4.

Delaunay simplices are geometrically dual to Voronoi polyhedra; that is, a vertex of a Voronoi polyhedron is the central site of the corresponding Delaunay simplex, and each site *p* (center of a Voronoi polyhedron) is a vertex of the corresponding Delaunay simplex (see, e. g. Okabe et al. 2000). The faces of the Delaunay simplices intersect the edges of the Voronoi polyhedra, and the faces of the Voronoi polyhedra intersect the edges of the Delaunay simplices. Delaunay simplices split up a Euclidean space into polyhedral cells as

well as a Voronoi diagram, but the Voronoi polyhedra are much less uniform, the number of faces varies from one cell to another (see Figure 3). Nevertheless, they have a different structure. The shape of a Voronoi polyhedron reflects the arrangement of all the neighbors of a given site. Delaunay simplices represent the structure of the clusters composed of four adjacent sites. As it was noted by Brostow (1998), Voronoi polyhedra and Delaunay simplex networks contain a formidable amount of information about the structure of the sample.

The Delaunay decomposition has been well known in the geosciences for many years, as one of the triangulated terrain models, see e.g. (Chen et al., 2003), (Mostafavi et al., 2003). Nevertheless, there are several useful properties of the Delaunay triangulation, which make it distinct from other triangulation methods. So, if the centers of the empty circles between pairs of adjacent triangles are connected, the Voronoi diagram is obtained. The construction of one automatically creates the structure of the other one, although these mutually dual procedures give fascinating but different insights into the structure of a set of points in d dimensions (Okabe et al., 2000), (Mostafivi et al., 2003).

Voronoi was the first one who noted the duality of these structures. However, it was his successor Boris *Delaunay* (originally Delone), who first defined the tessellation using the empty sphere method and presented it at the International Mathematical Congress held in Toronto, Canada, in 1924, in a paper, which was dedicated to the memory of Voronoi. Posteriorly, the dual of the Voronoi diagram got the notion *Delaunay tessellation* or *Delaunay triangulation*.

The Delaunay-Voronoi tessellation is widely used for modeling structures, which permit an interpretation as a dense packing of mono-sized spheres. In this case, the Voronoi cell or region is the polyhedron circumscribing a sphere. Medvedev and Naberukhin (1987) noted that the fundamental geometrical approach for describing the structure of random systems of atoms is based on Voronoi polyhedra and Delaunay simplices. In such systems, a Voronoi polyhedron of a given atom is a space region, all the points of which are closer to the center of the given atom than to the centers of the other atoms of the system. The interstices within a packing form a continuous network of interconnecting cells in a Voronoi diagram. Then, the geometry of a packing can be mathematically described, by the geometrical characteristics of the cells. The main idea is to construct a network of space-filling convex cells, where each cell contains exactly one sphere.

In material sciences, the Voronoi polyhedron is directly related to the connectivity of particles, like the thermal conductivity or interparticle forces, while the Delaunay cell is related to the connectivity of pores in a structure, e.g., permeability. The void space in a Delaunay tetrahedron corresponds naturally to a pore body in porous structures (Yang et al., 2006), (Gladkikh and Bryant, 2007) (Burtseva et al., 2015).

The reader can find detailed descriptions of Voronoi diagrams and Delaunay tessellations, e.g., in the works by Okabe et al. (2000), Langetepe and Zachmann (2006), de

Berg et al. (2008). For illustrations of Voronoi-Delaunay tessellations, the reader can consult the papers by Nolan and Kavanagh (1995), Okabe et al. (2000), Medvedev (2002), Chen et al. (2003), Langetepe and Zachmann (2006), Khirevich et al. (2011), Marchal (2011). Various algorithms for computing Voronoi-Delaunay diagrams were described in the works by Aurenhammer (1991), Okabe et al. (2000), Mostafavi et al. (2003).

3 The Voronoi diagram in Laguerre geometry

In the cases when the structures are composed of spheres with different radii, applying an ordinary Voronoi tessellation technique may provoke that the regions cut spheres or the adjacent elements are not necessarily in contact. It also produces errors during the estimation of the volume on each sphere and the number of faces on the polyhedron (Park and Shibutani, 2007). Therefore, as the spheres are not of the same size, a bisection cannot be the exact plane to represent the polyhedron, and the Voronoi-Delanay tessellation is not an appropriate method. Sugihara (2002) noted that there were various directions to generalize the Voronoi diagrams, where the Euclidean distance was replaced by a variety of distances, including the L_p distance, the convex distance, the additively and/or multiplicatively weighted distances and the boat-sail distance. Nevertheless, in generalized Voronoi diagrams some good properties have disappeared, particularly, the edges are converted into complicated curves in a generalized Voronoi diagram while they are portions of straight lines in the ordinary one.

One possible alternative is the *Voronoi diagram in Laguerre geometry* where a radius, or weight, is assigned to each particle. It is based on the power lines of neighboring (perhaps contacting) circles. Such a diagram is also referred to as the *radical* or *power diagram* in the literature, and it is an extension of the concept of the Voronoi diagram in the ordinary Euclidean geometry for n sites to the one in the Laguerre geometry for n circles of different radii in the plane, where the distance between a circle and a site is defined by the length l of the tangent power line.

Let $G = \{c_1, c_2, \ldots, c_n\}$ be a set of n circles in the plane $\mathbf{R}^2$, and let p_i and r_i, respectively, be the center and the radius of the circle c_i, $i = 1,\ldots, n$. For the point P and the circle c_i, the *Laguerre distance* between P and c_i is defined as follows:

$$d_L(P, c_i) = d(P, p_i)^2 - r_i^2,$$

where $d(P, p_i)$ denotes the Euclidean distance between P and p_i. According to the mathematical rules, the distance is the square from $d_L(P, c_i)$, but it is not taken in Laguerre geometry, to be defined even when the point P is inside the circle c_i, in which case the result of the subtraction in the above equation is negative. So, it is not a distance in a mathematical sense, it just defines a ‘degree of farness’ (Sugihara, 2002), (Bagi, 2006). Figure 5 shows the geometrical representation of the Laguerre distance.

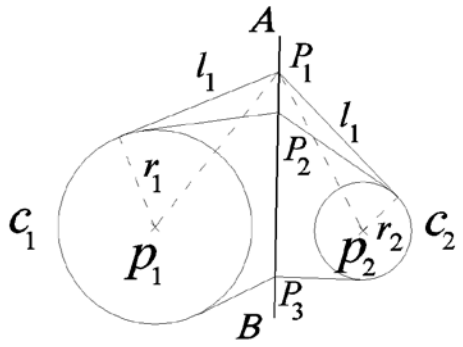


Figure 5. The geometrical representation of the Laguerre distance l between the circles c_1 and c_2 with the radii r_1 and r_2, and centers p_1 and p_2, respectively; the line AB is the radical axis of c_1 and c_2; every point P on AB is equidistant to the circles c_1 and c_2.

The possible mutual positions of the circles are illustrated in Figure 6 (Imai at al., 1985). The radical (power) line, also called *locus* or the radical axis of c_1 and c_2, is a straight line, which is perpendicular to the line connecting the two centers of the circles c_1 and c_2, and every point of this line is equidistant from c_1 and c_2 (Figure 6 a). If two circles overlap, their radical axis is the line connecting the two points of intersection (Figure 6 b). If one circle includes the other one, there is no distance between the circles (Figure 6 c). If three circles c_1, c_2 and c_3 intersect, and the centers are not on a line, then the three radical axes among c_1, c_2 and c_3 meet at a point, which is called the *radical center* of c_1, c_2 and c_3 (Figure 6 d).

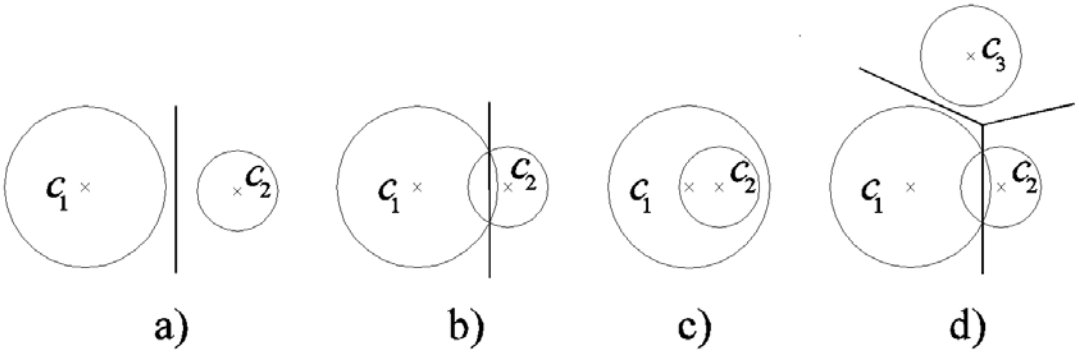


Figure 6. Radical or power lines of two a) separated, b) overlapped, c) included circles, and d) three circles.

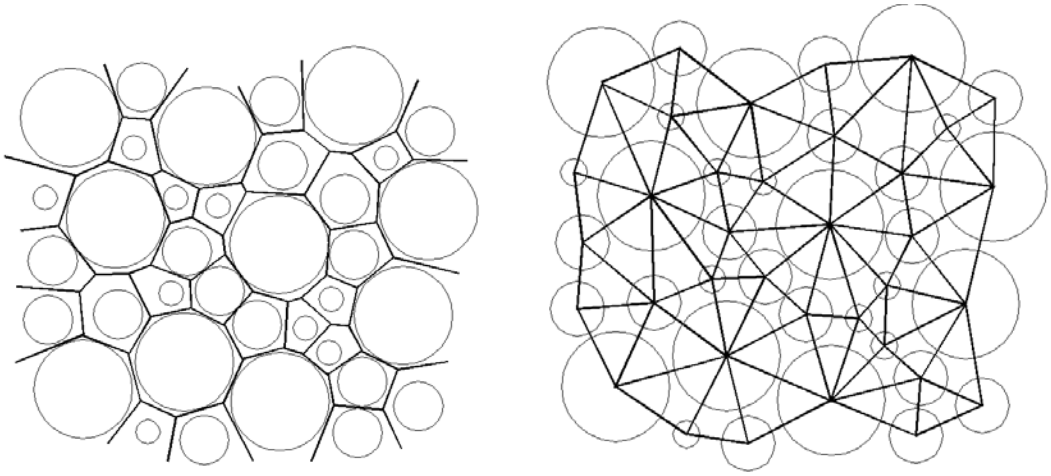
Each point on an edge is equidistant from exactly two sites, and each vertex is equidistant from at least three sites. Formally, the Laguerre Voronoi region for c_i is defined as follows:

$R(G; c_i) = \{P \in \mathbf{R^2} \mid d_L(\mathrm{P}, c_i) < d_L(\mathrm{P}, c_j), j \neq i\}$.

The plane is therefore partitioned into the regions $R(G, c_1)$, $R(G, c_2)$,…, $R(G, c_n)$ and their boundaries. Such a partition is called the Laguere-Voronoi diagram for G, and the elements of G are called the *generating circles*. So, if the generating circles are mutually disjoint, a point on an edge of the diagram has the tangent line segments with equal lengths to the associated two generating circles.

When performing this construction for every pair of spheres in the 3D space, polyhedral convex cells are generated. Similar to the Delaunay tessellation, the radical one divides the whole packing space into a set of non-overlapping convex polyhedra, each polyhedron contains exactly one sphere, and the touching spheres have a common face. For a more detailed description of Laguerre-Voronoi diagrams as well as for illustrations, the reader can consult the works by Imai et al. (1985), Sugihara (2002), Bagi (2006), Fan et al. (2004), Pottmann et al. (2015).

The Laguerre-Voronoi diagram is the dual to a regular triangulation and vice versa as well as the Delaunay cell is the topological dual to the Voronoi polyhedron. A 2D representation of a Laguerre-Voronoi tessellation for a set of multi-sized circles and the corresponding Delaunay network is given in Figure 7. The vertices of a regular triangulation are the circles (germs) of the corresponding power diagram, the edges correspond to the faces and the vertices of the power diagram are the orthogonal centers of the triangulation. A weight is similar to a distance and it enables some control of the size of cells. Larger circles (spheres in 3D) tend to have larger cells than smaller ones. If the radii of all circles in the set are equal (or all weights are equal), the Voronoi-Delaunay tessellation is obtained. The Delaunay and regular triangulations of the center points P verify the same ‘empty sphere’ property: no site falls into the interior of the circumcircle of any triangulation simplex.



a) b)

Figure 7. An example of a Voronoi diagram in Laguerre geometry for a set of multi-sized circles: a) Voronoi diagram; b) corresponding Delaunay triangulation.

At the moment, the 3D extension of a Voronoi diagram in Laguerre geometry should be the most powerful tool to model ensembles composed of multi-sized spheres. It may be also applied to solve effectively a number of geometrical problems such as those of determining whether or not a point belongs to the union of *n* circles/spheres, finding the connected components of *n* elements, or finding the contour of the union of *n* elements (Imai et al., 1985).

4 Packing of spheres

Any ensemble composed of spheres should be interpreted as a close, random or lose packing. The general properties of the packings composed of mono-sized spheres are now well known. The maximal *density* is reached by an ordered arrangement. In 1611, Johannes Kepler conjectured that the density of a packing of identical spheres is never greater than

$$\pi/(3\sqrt{2}) \approx 0.74048,$$

which is attained by a face-centered cubic close packing (fcc) or a hexagonal close packing (hcp) in a sufficiently large domain (Marchal, 2011), (Benabbou et al., 2010). It should be an upper bound on the density of the packing fraction.

The void fraction in a packing is referred to as the *porosity*. A random packing with highest density/lowest porosity is referred to as a random close packing (RCP), which by its nature is not totally random when the spheres do not overlap. No theory is provided about the exact value, but the well-accepted limit is 0.64±0.02 (Berryman, 1983), which is considered as the highest density for irregular arrangements of equal spheres in 3D. Random packings formed with no particular bias towards high densities have a density of around 0.58±0.2 depending on the packing assumptions (Onoda and Liniger, 1990). In a more recent publication, Zhang et al. (2006) affirmed that ordered structures can be reproduced in the range [0.2595 … 0.4764] of the void fraction, meanwhile disordered packings exhibit a much smaller porosity falling into the range [0.36 … 0.40]. These densities have been reproduced both in physical experiments and in computer experiments for mono-sized spheres (Burtseva et al., 2012). Nevertheless, there is no satisfactory theory describing either the density limits, or the geometrical properties of the structures containing polydisperse spheres.

The packing models should be classified into static, dynamic and constructive ones. *Static* models are designed to produce a fixed arrangement of spheres, whereas *dynamic* ones are capable of producing a sequence of arrangements. The simplest approach to simulate a static packing is a sequential addition of the particles to an initial configuration, e.g., using the Monte Carlo method (Luchnikov et al., 2002), (Medvedev, 2002), (Zhang et al., 2006). Physically a more realistic approach is a *dynamic* packing, where the particles

change their position and/or their size during the filling/reordering process (Mościński et al., 1989), (Yang et al., 2002), (Langetepe and Zachmann, 2006). Usually, such an algorithm involves three steps: (a) generate a set of particles either randomly or by a regular repartition, (b) check and eliminate all intersections, (c) apply the physical force so that the potential energy of each particle is minimal. The dynamic methods are very costly in terms of computing time. This is because the position and/or the size of each particle are frequently recomputed at each step of the filling process. The *constructive* techniques suppose only geometric calculations, and the position (and often also the size) of each particle are kept throughout the filling process (Benabbou et al., 2010).

Usually, the modeling of random packings is comprised of a sequential deposition of spheres under the influence of gravity, by dropping them from random locations, and allowing a sphere to roll until settling on the container bottom or top of three other spheres in a gravitationally stable position. Tessellation methods represent an alternative to this approach, because they are not based on the gravitation effect, meanwhile molecular dynamic laws are domineering on the micro- and nanolevels. Nevertheless, in recent works, one can observe that interparticle forces were included into diagram construction algorithms, e.g., the Jordey-Tory algorithm, the force-biased algorithm, the discrete element method (DEM) as well as their modifications (Mościński et al., 1989), (Benabbou et al., 2010), (Yi et al. 2012).

A Voronoi-Delaunay tessellation is widely used for modeling structures, which permit an interpretation as dense packings of mono-sized spheres, one of the more studied models in Mathematics. Such packings are characterized by a direct contact of spheres, described numerically by the coordination number $\langle C \rangle$, which is defined as the number of spheres touching everyone in the structure. For the mono-disperse case, its limit is known to be $\langle C \rangle = 12$, representing the limit of the faces of a cell in the corresponding Voronoi diagram. For real random close packings of equal spheres of density 0.62, it is evaluated to be equal $\langle C \rangle = 6.4$ (Bernal and Mason, 1960). A close packing reduces both the volume of the Voronoi cell and the size of the void, and hence significantly alters both the porosity and the permeability (Rogers at al., 1994). A packing model is related to the shape of the Voronoi polyhedron associated with the lattice formed by the centers of the spheres. For an ordered packing, each Voronoi polyhedron has the same size and shape for each sphere. For a random packing, the Voronoi polyhedra vary in size and shape.

In 1998, Mac Laughin has demonstrated that the smallest Voronoi cell is a regular dodecahedron circumscribing the sphere. For mono-sized spheres, the ratio of the sphere to the cell volumes is 0.754697, which is very close to Kepler's limit 0.74048 (Marchal, 2011). This ratio is considered as the best upper bound on the space occupation, and the tessellation as a convenient method to model a dense structure of spheres.

The properties of Voronoi cells are associated with the local packing density and the disorder. Initiated by Finney (1970), the approach has found an increasing use for

characterizing the morphology of random sphere packings. In particular, Schenker et al. (2009) investigating and comparing different methods to quantify the microstructural degree of heterogeneity of unconfined particulate packings as models for coagulated colloids found that the Voronoi volume distributions, i.e., the distributions of the volumes of the Voronoi cells in the tessellated packings, reflected microstructural differences between the packings better than other measures.

Initial arrangements of elements for tessellation goals can be obtained with different methods. So, they can be generated as a random set of particles. Some packing algorithms in a Voronoi diagram context were proposed by Oakeshott and Edwards (1992). A suitable method was suggested by Barbier et al. (2014). Intermediate cases between regular structures and random ones can be defined using a finite perturbation moving each site around its initial (regular) position according to the following relation:

$$s = s_0 + \alpha u,$$

where s is the position vector of the perturbed site, s_0 is the unperturbed position vector, u is a random vector, and α is a real positive number, called the perturbation coefficient, which characterizes the magnitude of the perturbation. The limiting case $\alpha = 0.0$ corresponds to a fully regular structure and $\alpha = 1.5$ is close to a true random structure.

Lochmann et al. (2006) applied a fast packing program, which used a force-biased procedure (Mościński et al., 1989). The initial configuration of that algorithm is characterized by a set of N spheres with random centers uniformly distributed in a cubic container and a specified radius distribution. Overlapping was permitted. While the number of spheres is fixed, the algorithm attempts to reduce overlaps between spheres by shifting overlapping spheres and gradual shrinking of the radii. This algorithm enables the simulation of random dense systems of spheres with arbitrary radius distributions and is able to generate packings with densities close to that of crystalline states for mono-sized spheres.

Yi et al. (2012) used the discrete element method (DEM) to generate a packing of a ternary mixture of spheres. The translational and rotational motions of each particle were described by Newton's second law of motion, where the gravity and interparticle forces as well as the torques were explicitly considered. Periodic boundary conditions were applied in two horizontal directions to eliminate the wall effect. To produce a stable packing, the particles were allowed to settle down, under gravity and all other forces considered, until their velocities are approximately equal to zero.

5 Tessellation methods for mono-sized spheres packings

The structures of the lattices generated by randomly packed mono-sized spheres was extensively studied over a long time period because of its importance as a predictive model

dealing with a wide range of assembles. The research was centered principally on measuring the packing properties and the acquisition of void distribution models. Utilizing a tessellation approach, the authors discussed also a convenient polyhedron shape. The tetrahedral tessellation, where the vertices of each tetrahedron are the centers of four neighboring spheres, is a useful method for modeling structures containing equivalent spheres. Other available methods mentioned in the related literature are square, triangular and hexagonal tessellations, which are composed of area-filling squares, triangles and hexagons, respectively (Chan and Ng (1988). The variants of the Delaunay-Voronoi tessellation describing the models for different structures, which were found in the literature, are reviewed below.

In the works by McGeary (1961), Mason (1971), Chan and Ng (1988), Zou and Yu (1995) and Van Antwerpen (2010), a random packing of equivalent spheres is described in terms of a tetrahedral tessellation. The selection of a tetrahedron as the basic unit in these studies was grounded on the known observation that the average coordination number of a random packing of equal spheres is about six, with three on the top and three on the bottom. Such tetrahedra are related to Voronoi polyhedra. Each face of the Voronoi polyhedron contributes one edge to the network of the tetrahedron.

McGeary (1961) described a ball-bearing model in terms of tetrahedral subunits in random close packed lattices of uniform spheres. Zou and Yu (1995) and Van Antwerpen (2010) analyzed the voids associated with tetrahedral structures. Each tetrahedral structure contained a central pore and four outer constrictions. Although the four connections associated with each pore varied in their sizes, nevertheless the pores joined by a common constriction were similar in their size.

Studying the drainage of a liquid from porous materials, Mason (1971) highlighted two principal concepts concerning the material: there is a network of interconnections within the material, comprised of pores defined as small regions of that network. Some materials, for example, foams can be very highly interconnected. The capillary properties of such pores define the capillary pressures and in isolation from the network, they determine whether the liquid can fill or drain an individual pore. In a random sphere packing, the most convenient pore is a tetrahedral subunit formed by joining the centers of neighboring not necessarily touching spheres together. A method for generating these tetrahedra was given. Some capillary properties of the assembly were derived using an approximation for the draining and filling curvatures of the pore spaces.

Arzt (1982) combined the concepts of the radial distribution function and the Voronoi polyhedron to investigate the densification of a powder. Analytic expressions for the contact number and the contact area as functions of the relative density were derived. The short-range redistribution and long-range redistribution on the process of compaction and sintering were explicitly considered.

Chan and Ng (1988) applied a tetrahedral tessellation to a computer-generated random packing of nearly equal spheres confined in the pore chambers. The objective was to identify the tetrahedral pores and then to determine the geometrical characteristics of the pore space. The tessellation procedure began with a seed tetrahedron. Then, in a crystal growth-like manner, tetrahedra were added one at a time to the seed until a cluster of non-overlapping, space-filling tetrahedra was formed. Each tetrahedron had a pore chamber and four constrictions, one on each of its four triangular faces. A simulation algorithm was proposed. A statistical analysis allowed the determination of various correlations among the pores and constrictions.

Nolan and Kavanagh (1995) applied the Voronoi-Delaunay tessellation technique, which was able to predict accurately the transport properties of the porous medium for an ordinary diffusion. The authors compared the distribution of pore polyhedra in a random close packing of equal-sized spheres obtained using a computer simulation with experimental data obtained by previous works. The analysis of the results suggested that the structure of a random close packing is characterized by irregular octahedral and planar configurations rather than tetrahedral as previously thought.

In the paper by Yang et al. (2002), the topological and metric properties of Voronoi polyhedra for uniform fine spherical particles were analyzed and facilitated by the Voronoi tessellation. They were quantified as a function of the particle size and the packing density. The authors have shown that the average sphericity coefficient of the Voronoi polyhedra varied with the packing density. Moreover, with decreasing the particle size or the packing density, the average face number of the Voronoi polyhedra decreased, and the distributions of the face number and the edge number became broader and more asymmetric; the average perimeter and the area of the polyhedra increased, and the distributions of the surface area and the volume of the polyhedron become more flat and can be described by the log-normal distribution.

Two problems were addressed in (Luchnikov et al., 2002) for the analysis of the free volume, considering the packing of balls confined in a cylinder: 1) an efficient construction of the confined Voronoi diagram inside a cylindrical boundary, and 2) an analysis of the Voronoi network to study the distribution of the empty spaces (voids) in the system. The way used was based on the idea of the Delaunay empty sphere, which moves inside the system so that it touches at least three objects at any moment of time. In this case, the center of the sphere moves along an edge of the 3D Voronoi network. If the distance from any point in the space to any object is expressed by explicit functions d, then the trajectory of the center of the Delaunay empty sphere can be computed numerically by performing a series of small shifts along the edge. The direction of the shift v was found from the equation:

$$(\nabla d_i \cdot v)|_r = (\nabla d_j \cdot v)|_r = (\nabla d_k \cdot v)|_r,$$

where the indices *i, j, k* enumerate the objects touched by the sphere. This approach was implemented in the three-dimensional space and tested on the models of a disordered packed bed of 300 balls in cylinders of different radii. The algebraic solution for the empty sphere problem was given. Two models were built by means of the Monte Carlo relaxation method.

The work by Yang et al. (2006) presented a numerical study of the pore structure of fine mono-sized particles by means of a granular dynamics simulation. The pores and their connectivity were then analyzed in terms of the Delaunay tessellation. The geometries of the pores were represented by the size and shape of the Delaunay cells and quantified as a function of the packing density or the particle size. It was shown that the cell size decreased and the cell shape became more spherical with increasing the packing density. A general correlation existed between the size and shape of the cells: the larger the cell size relative to the particle size, the more spherical is the cell shape. This correlation, however, becomes weaker as the packing density decreases. The distribution of the equivalent volume diameter of the Delaunay cells for different packing densities was studied. The size distribution of the Delaunay cells was described by the lognormal distribution. A formula for the probability function was given. The pore scale information would be useful to understand and model the transport and mechanical properties of porous media.

In a series of three papers by Song at al. (2010), Wang et al. (2011), Briscoe et al. (2010), the authors studied the jamming effect on granular materials and emulsions in terms of a random close/lose packing using Voronoi diagrams for a mathematical and statistical analysis of the structures.

Song at al. (2010), introduced a “Hamiltonian”-like function, called the volume function, to describe ensembles of jammed matter from a geometrical point of view. In the jammed systems, such as granular materials and emulsions, the volume function represents the available volume of each particle. At the microscopic level, the observed space was partitioned into a set of regions, associating all grain centroids in each region to the closest grain centroid, and so the volume function was interpreted in terms of the Voronoi volume associated to each particle. The Voronoi volume was used to tile the total system volume, and it replaced energy as the conserved quantity in a new micro-canonical ensemble for a jammed granular matter.

An analytical formula, valid for any dimension *d*, was provided for the Voronoi volume in terms of the contact network, basing on a formal expression for the volume of the Voronoi cell of particle *i* moving in the direction $\hat{s}$:

$$w_i^{vor} = \oint \int_0^{l_i(\hat{s})} r^{d-1}\, dr d\hat{s} = \frac{1}{d} \int \left(\frac{1}{2R} \min_j \frac{r_{ij}}{\cos\theta_{ij}} \right)^d \mathrm{d}\hat{s} = \frac{1}{d} \oint l_i(\hat{s}) d\hat{s},$$

where r_{ij} is the distance between the positions of the particles *i* and *j*, the integrand is over all the directions $\hat{s}$ forming an angle θ_{ij} with $\vec{r}_{ij}$, and *R* is the radius of the grain; $l_i(\hat{s})$ is

the limit of the distance from the particle i to the boundary of its Voronoi cell in the $\hat{s}$ direction:

$$l_i(\hat{s}) = \min_j l_{ij}(\hat{s})/2\cos,$$

where

$$l_{ij}(\hat{s}) = r_{ij}/2\cos\theta_{ij}.$$

This formula is valid independently whether the particle j is in contact with i or not. It was presented in more detail in subsequent papers. A statistical theory was developed for the probability distribution of the volumes in 3D to calculate the average volume function coarse-grained at a mesoscopic level. It was discovered that the mesoscopic volume function is inversely proportional to the coordination number.

In (Wang et al., 2011), the authors combined an extended statistical mechanics (Edwards' approach), where the role traditionally played by the energy and temperature in thermal systems was substituted by the volume and the compactivity, with a constraint on the mechanical stability imposed by the isostatic condition, to use a relation between the local Voronoi volumes of the constituent grains expressed by the volume function and the number of neighbors in contact. This permitted the authors to simply combine the two approaches to develop a theory of volume fluctuations in a jammed matter. These results lead to a phase diagram that provides a unifying view of the disordered hard sphere packing problem and further sheds light on a diverse spectrum of data, including the random lose packing state.

In a third paper by Briscoe et al. (2010), the authors characterized randomness in disordered packings of frictional and frictionless spheres using the theory and simulations of identical spherical grains. The entropy of the packings was defined through the force and volume ensemble of a jammed matter, basing on the Voronoi-Delaunay approach. A mesoscopic ensemble of isostatic states was then utilized in an effort to predict the entropy through the definition of a volume function that was dependent on the coordination number.

In the works by Khirevich et al. (2011) and Khirevich et al. (2012), the Voronoi-Delaunay tessellation was used for the analysis of the mass transport properties and the morphology of different packing structures. Khirevich et al. (2011) have shown that the combined influence of the bed porosity and the packing protocol on the morphology of an unconfined random sphere packing was captured by the second and third statistical moments (standard deviation and skewness) of the Voronoi volume distribution of the packing. In the work by Khirevich et al. (2012), topological information was derived from the radial profiles of the statistical moments of the free Voronoi volume (V_{free}) distributions, where V_{free} is the difference between the volume of a Voronoi cell and the volume of the contained sphere. A uniform grid was used to simulate the flow and the dispersion and to determine the interparticle porosity profiles. The radial profile of the standard deviation of these V_{free} distributions, $\sigma(V_{free})$, in the form of an integral measure

was identified as a quantitative scalar measure for the transcolumn disorder. The identified measure strongly correlated with the resulting eddy dispersion in the packings. The success of this measure lay in its ability to account for both, the packing density and the disorder, and thus to distinguish between packings that were quite similar in one respect (e.g., their radial porosity distributions), but different in another one (e.g., their disorder).

With the use of monochromatic null ellipsometry and scanning electron microscopy techniques, the initial stages of palladium nanolayer growth were studied in (Kuchumov et al., 2013). The analysis of electron microscopy images of growing film surfaces was based on the Voronoi–Delaunay method with the introduction of parameters such as peak, valley and minimum spanning tree (MST). The parameters used directly reflected the process of film growth, whereby two stages of the process have been distinguished. The dynamics of film growth (including the dynamics of changing the number of shades) were described by changing the Voronoi diagrams in the course of film growth. These changes were characterized by two parameters: the number of vertices (centers of the polygons) and the total length of the lines (valley) in the Voronoi diagram. As an indicator of the total length of the lines a category of the MST was used, whose total length of graph ribs was minimal. It was defined as an undirected graph without cycles that contains all the nodes of the network (graph junctions).

Studying the virtual polycrystalline grain structures with cohesive boundaries for large-scale crystal plasticity finite element (CPFE) analyses, Zhang at al. (2012) used the controlled Poisson Voronoi tessellation (CPVT) model to generate virtual grain structures that were statistically equivalent to metallographic measurements in terms of the grain size distribution. A grain boundary representation scheme was proposed to produce cohesive interfaces for Voronoi tessellations and automatically partitioning multiple junctions. The authors used a non-local parameter α to evaluate the regularity of a Voronoi tessellation defined by:

$$\alpha = \delta / d_{reg},\ 0 \le \alpha \le 1,$$

where δ is a control parameter and d_{reg} is the distance between two adjacent seeds in an equivalent regular tessellation, i.e., a regular hexagonal tessellation for a 2D Voronoi tessellation or a regular truncated octahedral tessellation for a 3D structure. When $\delta = d_{reg}$, $\alpha = 1$ represents a regular tessellation, and $d < d_{reg}$, $\alpha < 1$, corresponds to an irregular tessellation. As the regularity d decreases, Voronoi tessellations become more disordered. If $\delta = 0$, the Voronoi tessellation is a completely random tessellation, i.e., it is of the Poisson type. Gamma distribution functions and lognormal functions have been widely used to fit grain size distributions of Voronoi tessellations.

6 Modeling complex mixture structures using tessellation methods

The use of Voronoi diagrams in Laguerre geometry is an appropriate method for studying and modeling packings of multi-sized spheres. In this section, we give a brief review of the works applying tessellation techniques to model and study structures, which contain multi-sized components, focusing mainly on the mathematical aspects of the tessellation method used and on a specific particle size distribution, which is considered as the more significant factor when the resulting structure is analyzed. For illustrations, see, e.g., Fan et al. (2004), Lochmann et al. (2006), Redenbach (2009), Wu et al. (2010), Yi et al. (2012), Rycroft (2013).

The research in this area was mainly centered on studying the volume and topology parameters, such as the number of cell faces and edges per face, the surface area and the volume per polyhedron for different size distributions. The latest publications showed several advances in mathematical and computational tools applied to the modeling and analysis, such as

- Employment of specific statistics, e.g. correlations between the number of faces per cell and the coordination numbers (Lochmann et al., 2006), the coefficient of variation of the volume distribution (Redenbach, 2009); the dependence of the geometric characteristics of the cells on the volume fraction, the moments of certain cell characteristics (Redenbach, 2009);
- Embedding of the molecular dynamic forces (Antwerpen et al., 2010), (Benabbou et al., 2010), (Khirevich et al., 2011), (Park et al., 2012), the effect of jamming (Briscoe et al., 2010), (Song et al., 2010), (Wang et al., 2011), elastic stress field fluctuations (Lavergne et al., 2013); hydrodynamic correlation (Khirevich et al., 2012);
- Use of specific methods, as the intercept count method to study the stereology of diagrams (Wu et al., 2005), Richards's method as an alternative way to calculate the distance between the atoms (Park and Shibutani, 2007);
- Introduction of new parameters, e.g., Kelvin's parameter for foam materials; new strategies in geometrical modeling methods (Benabbou et al., 2010), (Hardenacke and Hohe, 2010), particle relocating algorithms (Wu et al., 2010), (Lochmann et al., 2006).

In the paper by Fan et al. (2004), the Poisson-Voronoi diagram was considered using the Laguerre-Voronoi approach. The Poisson-Voronoi diagram is a kind of a Voronoi diagram with the set of points generated through a homogeneous Poisson point process. A Poisson-Voronoi diagram is composed of an array of convex, space-filling and non-overlapping polyhedra, which represent the grains of the polycrystalline material. A polyhedron of the Poisson-Voronoi diagram possesses the properties that four edges share a vertex and three faces share an edge, which are also observed in a real material. Fan et al. (2004) proposed a model called the Voronoi diagram in Laguerre geometry based on a random close packing of spheres (RCP-LV) diagram, which was probably better than the Poisson-Voronoi

diagram in the simulation of the microstructure of real polycrystalline materials because it was based on real material characteristics instead of inadequate ones used in the Poisson-Voronoi diagram: the average number of faces per polyhedron, the range of the coefficient of variation of the grain volumes, and the volumes of the polyhedra obeyed a lognormal distribution instead of a gamma distribution.

A conclusion of the work by Wu et al. (2005) was also that the RCP-LV was a better representation of a polycrystalline structure than the conventional Poisson–Voronoi diagram, where the coefficient of variation of grain volumes (CVg) was selected close to real materials. The stereology of the RCP-LV diagram was investigated with a lognormal-like volume distribution by an intercept count method. A problem, discussed by the authors, was how to recover detailed spatial structural information from stereology measurements. A possible solution was presented in the paper: by varying the volume distribution of the spheres in a random close packing, various series of RCP-LV diagrams can be constructed and their spatial and stereological data can be accumulated simultaneously.

An application of tessellation-based methods, which includes an analysis of the correlations between the cell face and the coordination number, was proposed in the paper by Lochmann et al., (2006). In this paper, the radical (Laguerre-Voronoi) tessellation was employed. The authors applied a fast packing program, which used a so-called force biased procedure for the initial configuration. An analysis of the geometrical organization of disordered packings of spheres with different statistical methods was performed. Four different structures were considered: mono-sized, binary, power-law and Gaussian size distributions. A comparison of the basic geometrical characteristics such as the packing fraction, the two-point probability function, the pair correlation function and the coordination number has shown that these characteristics can have quite different forms, which are closely related to the radius distribution. The description was refined by means of tessellation-related characteristics, which enable a quantitative description of the different local arrangements by means of the number of cell faces and edges per face. An in-depth analysis of the coordination number, which is the fundamental topological parameter, was given for different radii distributions.

Park and Shibutani (2007) applied a weighted Voronoi tessellation technique to the study of the internal structure of metallic glasses using Richards's method, a kind of a weighted Voronoi tessellation technique. Richards suggested an alternative way to confirm that the ratio of the distance between the atoms on the plane equals the ratio of the atomic radii.

In the paper by Redenbach (2009), Laguerre-Voronoi tessellations generated by random sphere packings were employed as models—for the microstructure of cellular or polycrystalline materials, using lognormal or gamma distributions of the volumes, because these distributions were often suggested for the size distributions of grains (cells) in granular (cellular) materials. The Laguerre cells on the volume fraction in the sphere

packing and the coefficient of variation of the volume distribution were studied in detail. The authors investigated the dependence of the geometric characteristics of the Laguerre cells on the volume fraction in a sphere packing and the coefficient of variation of the volume distribution. The moments of certain cell characteristics were described by polynomials, which allowed the author to fit tessellation models into the modeling of real materials, such as open polymer and aluminum foams, without further simulations. The author considered relatively dense packings with 66.7%, where the cell volumes, as well as the sphere volumes, were approximately log-normally distributed. The topology parameters, the number of facets per cell and the number of edges per facet and their tessellation characteristics were analyzed. The procedure was illustrated by the examples of open polymer and aluminum foams.

The paper by Benabbou et al. (2010) dealt with a geometrical modeling of granular structures basing on power diagrams. A simple method was proposed to transform the generated structure with spherical balls into a diagram of polyhedral grains closer to the reality. It was performed in two steps: 1) the construction of the weighted Delaunay triangulation of the centers of the particles. In this triangulation, the weight W_i of point P_i is

$$W_i = P_i + Gb(R_i),$$

where R_i is the radius of the particle centered on P_i and $Gb(R_i)$ is the thickness of the grain boundary around this particle; 2) the Laguerre or power diagram, which is the dual of the built triangulation, was considered. In the obtained diagram, each cell contains a particle as well as the grain boundary that surrounds it. To separate the grain boundaries, the obtained cells must be isotropically shrunk. From the vertices o_i of a cell and the point P, which is the center of the corresponding particle, the vertices $\tilde{o}_j$ of the shrunk cell were defined by:

$$\overrightarrow{P\tilde{o}_j} = (\frac{R}{W})\overrightarrow{P\tilde{o}_j}.$$

The grain sizes were randomly determined in the specified distribution, and their repartition was defined by a proposed constructive advancing-front algorithm.

Hardenacke and Hohe (2010) investigated structural solid foams with an irregular random microstructure due to a large cell size. The study included strategies of the Voronoi tessellation, both in its direct Γ-form with spatially uncorrelated nuclei and in its δ-version with a minimum distance between neighboring nuclei, for the division of the space in the generation of computational models of the microstructure of solid foams and a numerical analysis of their properties. The Γ-distribution of the cell size was selected instead of the usual logarithmic normal distribution, and the minimum distance

$$\delta \leq r(p_i, p_j),\ i \neq j,$$

was introduced to avoid unrealistic shapes. The technique of a close packing of spheres in conjunction with a Voronoi tessellation in Laguerre geometry was used as an alternative. The basic idea of this procedure was the use of the nucleation points r_i with an associated

circumcircle of radius r_i^*. The prescribed associated radii r_i^* defined non-intersecting circles (or spheres in the three-dimensional case) surrounding the nucleation points p_i. Hence, the minimum distance satisfies the inequality was:

$$r_i^* + r_j^* \leq r(p_i, p_j),\ i \neq j.$$

Formulas for calculating some principal statistics were also given. Some procedures for the smoothing and optimization of the Delaunay triangles were proposed. The objective of the optimization was an improvement of the microstructure with respect to their energetic performance in terms of Kelvin's parameter for solid foams:

$$K_i = \frac{S_i}{A_i},\ i = 1,...,n.$$

where A_i is the i-cell area, and S_i is the total length of the line segments forming the individual cell i. Hence, the objective was

$$K_{\text{avg}} = \frac{1}{A_{\text{RVE}}} \sum_{i=1}^{n} S_i \rightarrow \min,$$

where Kelvin's parameters K_i of the individual cells are weighted with the areas A_i of the corresponding cells normalized with the average cell area A_{RVE}/n. The two-dimensional foam model considered can be generalized to the three-dimensional case in a straight forward manner.

A Laguerre-Voronoi tessellation based on a random close packing of spheres was performed by Wu et al. (2010). The authors considered this method as a successful one for modeling and characterizing two-phase composites. First, it was generated with two groups of spheres and each group had its own volume distribution, basically lognormal, by using a modified rearrangement algorithm. Then a Laguerre-Voronoi diagram was performed basing on the sphere packing to generate the grains of the two phases, thus the model of a two-phase composite was obtained. Various geometrical and topological characterizations were conducted, yielding useful information about this kind of composite. Three groups of representative parameters were selected to characterize the particle shape, the local and the overall geometrical distributing patterns: 1) the form factor (FF) to characterize a 3D grain shape; 2) the nearest neighbor distance (NND), and 3) the second order intensity function and the pair distribution function.

The FF was defined as follows:

$$FF = \frac{36\pi V^2}{SF^3},$$

where V and SF correspond to the volume and the surface area of a grain, respectively. The less the FF of a grain is, the more its shape deviates from a sphere. The NND was defined as the minimum distance from a grain to its nearest neighbor. A second order intensity function $K(r)$ was employed to describe the statistics of a spatial distribution. It was defined

as the expected number of points of interest lying within a distance r of an arbitrarily located point, divided by the point density:

$$K(r) = \frac{S_c}{N^2} \sum_{k=1}^{N} \frac{I_k(r)}{R_p},$$

where S_c is the volume of the finite cuboid C, N is the number of points selected in C, $I_k(r)$ is the number of points inside the sphere with its center at the point k and its radii r, and R_p is the edge effects correction, obtained as the ratio of the face area of the sphere with the radius r inside C to the entire face area.

Once $K(r)$ was obtained, the pair distribution function $G(r)$ was evaluated and used to quantify the likelihood of the occurrence of near neighbor distances:

$$G(r) = \frac{1}{4\pi r^2} \frac{dK(r)}{dr},$$

Three kinds of such a function *K(r)* were discussed in the experiments.

Three aspects were selected as general descriptions of the composite models: 1) the volume fraction of constituent phases; 2) the mean and standard deviation of the grain volume; 3) the grain volume distribution. Several topological parameters were computed. The authors concluded that the model and the characterization based on a random close packing of spheres using a Laguerre-Voronoi diagram are effective for analyzing a composite microstructure.

In the work by Park and Shibutani (2012), the composition of a binary system model was varied to compare the radical plane method, which considers the size of atoms, with the ordinary Voronoi tessellation technique. The results indicated that the error between these two analytical methods is large. Such errors were not simply a matter of quantity, but they can affect the entire analysis, for example, of the Voronoi polyhedron index. The results showed that a Voronoi analysis that did not consider the size difference of the atoms can lead to totally incorrect results.

In the paper by Yi et al. (2012), the packing structures for ternary mixtures were analyzed by a radical tessellation. The generation of the radical tessellation in the present work was facilitated by an open source program Voro+ developed by Ch. Rycroft (2013). The metric and topological properties of each polyhedron were studied as a function of the volume fractions of the constituent components. The studied properties included the number of edges, the area and the perimeter per radical polyhedron face, and the number of faces, the surface area and the volume per radical polyhedron. The properties of each component of a mixture were shown to be strongly dependent on the volume fractions. The authors concluded that the radical tessellation can be successfully used to model different properties of multi-sized packings and the development of a predictive method to describe the effect of the particle size distribution on the structural properties of the packing of particles. The authors noted that the structural results based on the Voronoi or radical

tessellation were increasingly used in the literature and gave some examples of these results.

Laguerre-Voronoi diagrams were used in the paper (Lavergne et al., 2013) to study the relation between the grain size distribution, the elastic stress field fluctuations and the description of incipient plasticity in polycrystals. A numerical scheme was used for the generation of polycrystalline microstructures. It combines the Lubachevsky-Stillinger algorithm (Lubachevsky and Stillinger, 1990) for a dense sphere packing with power diagrams. It has been shown that the combination of a dense-sphere packing and Laguerre-Voronoi diagrams provides a convenient way to produce microstructures with a prescribed grain size distribution.

In (Hitti et al., 2012), a generic statistical virtual microstructure builder in a finite element context has been introduced. The techniques in this generator were based on Laguerre tessellations. The authors used the Laguerre Tessellation Method (LTM), which consists in assigning a radius, or a weight, to each nucleus with no intersections between the created spherical particles, building the corresponding weighted Delaunay triangulation and then constructing its dual, the Laguerre tessellation. Spherical particles (powder) were generated with uniform and Gaussian distributions.

In the study by Wejrzanowski et al. (2013), a model based on Laguerre–Voronoi tessellations was used to simulate the geometry of engineering foams with log-normal size distribution. Geometrical features of the modeled foam structures, such as the number of faces per pore, delivered results close to the ones observed experimentally. This model permits the study of the variation coefficient effect on the pore size in foams. The results showed that a higher diversity in the pore size results in a reduction of the average number of faces per foam cell. It was found that this parameter varies from 13.7 to 14.5 for different pore size variation coefficients. Compared to the structures obtained via Poisson–Voronoi tessellations, where the number of faces per cell is about 15.5, the Laguerre–Voronoi approach gave results, which are closer to the real ones.

The topic of the work by Barbier et al. (2014) was the estimation of the variations in the mechanical behavior of Voronoi closed-cell foams of low relative density as functions of their microstructure. The authors employed intermediate cases between regular structures and random structures using a finite perturbation. New laws were proposed in order to approximate the macroscopic mechanical behavior of Voronoi closed-cell foams under uniaxial tension and compression.

An extensive and in-depth review by Randrianalisoa and Baillis (2014) was given for the traditional and recent advanced modelling approaches thermal conductive and radiative properties of solid foams with open-and-closed-cells. They found that the Laguerre–Voronoi tessellation carried out on a dense packing of spheres was a potential candidate for modelling and designing highly porous foams. Powerful models combined 3D foam modelling (by X-ray tomography, Voronoi tessellation method, etc.) with a numerical

solution of the transport equations. The authors concluded that the analysis of reconstructed 3D samples obtained from the Laguerre–Voronoi tessellation permitted to determine the topological information needed to feed analytical thermal models.

Vecchio et al. (2014) enriched the geometric characterization of Laguerre tessellations by computing the angles between the facets and the angles between the edges applied to foam materials. The authors investigated how the distributions of these features depend on the model parameters. For a known tessellation and a cell C, the authors defined the dihedral angle θ_e at edge e as the angle between the two facets of C sharing e:

$$\theta_e = \pi - \arccos(n \cdot m),$$

where n and m are the outward unit vectors normal to the two facets in C adjacent to e and $(\cdot)$ is the scalar product.

The other angles to measure were the ones between two edges on a facet, which were referred to as interior or bond angles. These angles can be measured via the scalar product of the direction vectors of the adjacent edges. The authors found that the mean value and the standard deviation of the angles were highly influenced by the parameters determining the sphere packing. In tessellations with a small degree of polydispersity (almost mono-disperse), the angles were distributed closely around the equilibrium. The authors concluded that Laguerre tessellations fitted to the observed microstructures according to cell volume, surface area, mean width and number of facets per cell proved to be able to capture the distribution of the angles.

7 Conclusion

The tessellation approach based on Voronoi diagrams is a powerful method to model and study sphere packings with a variety of problem assumptions. The basic tessellations are the Voronoi-Delaunay and the Laguerre-Voronoi ones, for mono-sized and multi-sized sphere size distributions, respectively. Aurenhammer (1991) and Yao (2002) also reviewed several kinds of a generalized Voronoi diagram, where certain features point out potential applications and can be crucial in future research.

A review of recent publications shows that the tessellation approach is an indispensable technique to model and study modern structures, whether in material science, powder technology, or in architecture. Although this approach is really not new, meanwhile its intensive use and, consecutively, a systematical study started around 2000 with advances in nanoscience and nanotechnology. The development of the tessellation methods has received a noted impulse with the application to the creation and study of foam materials, meanwhile crystallography is a typical application area. The related literature of the recent years shows a remarkable progress in the use of tessellation methods for the study of the effects of the packing properties for different particle size distributions on the density of

confined nanoporous structures, such as the shape, the topology, and thermodynamic characteristics. Therefore, Voronoi statistics, such as the number of cell faces and the edges per face, the surface area and the volume per polyhedron as well as specific distributions of the particle sizes, appear as typical characteristics of a structure. The research interest area is the correlation of the structure of a material with its properties and their optimization.

On the other hand, the high relevance of tessellation ideas to model different structures prorogues a progress in the mathematical background. The researchers propose new statistical and mathematical tools to bring more realistic factors into the models, such as correlation statistics, embedding the effects of the molecular thermodynamic or the gravity field, the use of specific packing algorithms and calculation methods, etc. Nevertheless, it is a wide area for future research, primarily with respect to the mathematical aspects.

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