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About the Delaunay–Voronoi Tesselation

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The topological description of the neighborhood of the constituing atoms in a dense random material (liquids, glasses) is of a major importance for their characterization. We discuss an algorithm for the Delaunay construction which is global and independent of the dimension of the space and derive from it the full dual Voronoi tesselation by an original realization of duality.

1. INTRODUCTION

An intense interest, experimental and theoretical, is devoted to random dense materials (liquids [1], metallic glasses, glasses [2]). These materials possess no long-range order, but a rather extended short-range order constrained through the packing; and their packing fraction can be quite as high as the densest regular lattices. The experimental diffraction measurements (X ray, neutrons, ...) allow one to determine the radial distribution function (RDF) of these materials, (i.e., the angular averaged density correlation function $\phi(r)$

$$\phi(\mathbf{r}) = \langle \rho(\mathbf{r})\, \rho(\mathbf{r}+\mathbf{r}') \rangle_{\mathbf{r}'}. \tag{1}$$

One may refer to reviews [2], or lecture notes [3]. This information is often insufficient to explain the properties of these materials; therefore, efforts have been made in several ways to build models providing a better insight into the structure of dense random materials.

In the following, we will restrict our discussion to materials for which the models of dense packing of random spheres with rather isotropic interactions between atoms are adequate. Bernal [4] has been a pioneer in this domain, building ball and stick models, and later computer models. The smallest densely packed cluster of identical hard spheres is a regular triangle in the plane (dimension 2), a regular tetrahedron in dimension 3, and, more generally, a d-dimensional simplex. This local unit is a seed of icosahedral symmetry, which cannot tile the Euclidian 3D space [5] in a simple way. This frustration leads to the disorder and the amorphous structures.

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Bennett [6] proposed an algorithm which simulates the growth of amorphous materials by condensation of atoms from the vapor phase onto a growing seed, obeying the local regular tetrahedral symmetry. In order to avoid dendritic growth, the adsorption site selected for condensing the atom from the vapor phase is the closest "pocket" from the center of the cluster. A pocket is a void or cavity in or on top of the condensed cluster, where it is possible to insert a new atom in close contact with its neighbors. Let us mention other authors which used and developed this class of algorithms [7–10], with or without a relaxation of the structure obtained by a partial minimization of the total energy of the system (described usually by pair interactions between atoms). This algorithm suffers from the defect that the density of the material is inhomogeneous and decreases with the size of the cluster.

Other classes of algorithms use the generation of a random cluster with prescribed density by sowing nonoverlapping atoms in a predefined volume and then performing relaxations of density and positions of the atoms as quoted above [11].

On the other hand, the molecular dynamics models simulate the formation of glasses by rapid quenching from the melt [12]. However, the quenching rates realizable on a computer are several decades higher than those attainable experimentally.

It is also possible to form amorphous materials by introducing a sufficiently high density of linear defects into a perfect material [13].

There exist now, also, deterministic models for these classes of materials, based upon the argument originally given by Sadoc [14], that perfect packing of regular tetrahedra could be achieved on curved space manifolds (the regular $\{3\ 3\ 5\}$ polytope on the sphere S^4, see Coxeter [15]).

The flattening process to the frustrated 3D Euclidian space [16] introduces a network of linear defects (dislocations and disclinations) discussed by Nelson *et al.* [17, 18]. Closely related, the quasiperiodic icosahedral phases alone become a subject of intense activity [19–24].

Once the geometrical positions of the atoms in space are known, the Voronoi construction [25, 26] provides a full description of the topological neighborhood of an atom and a simple covering (honeycomb) of the space. Numerous computer implementations have been proposed recently [27–29].

The dual Delaunay [18] construction [30] has been implemented in the case of liquids in [31, 32], and the corresponding algorithm published [33]. It is one of the most efficient; this is due to the fact that the Delaunay cells are perfect simplices in general, whereas the Voronoi cells are general convex polytopes, which belong to the class of simplicial complexes [34].

Our aim in this paper is to propose an algorithm which works in any dimension, even for manifolds. It performs the global Delaunay construction in any dimension; its main virtue is to give also a constructive way to realize the duality between both honeycombs and to use it in order to derive the whole Voronoi tesselation by inspection. This seems to be a new result, which also achieves a breakthrough for the computational aspects of this problem. It may be used independently of our realization of the Delaunay tiling; it avoids the construction of a Voronoi cell as the convex hull of its vertices. Both phases the Delaunay tiling and the Voronoi tiling are global and thus vectorizable; it constitutes therefore a progress over the sequential approaches [35, 36]. Our realization of the Delaunay tiling is merely a generalization of the work of Ogawa *et al.* [33] to any dimension and a simplification of their multiphase algorithm into one phase. It has therefore improved performances, even for the realization of the Delaunay tiling itself. But we hope that our construction of the Voronoi tesselation by an original implementation of duality will be appreciated as real progress.

Let us mention also that even though our introduction is centered in the field of amorphous materials, these constructions are also pertinent in many other fields of science (astronomy, geology, biology), as quoted in [33].

2. Definition of the Voronoi and Delaunay Dual Tesselations

A point $\mathbf{x}$ belongs to the Voronoi cell of atom i located at position $\mathbf{x}_i$ if it is closer to $\mathbf{x}_i$ than to any other point j of the system

$$\mathbf{x} \in V_i \Leftrightarrow |\mathbf{x} - \mathbf{x}_i| \leqslant |\mathbf{x} - \mathbf{x}_j|, \qquad \text{whatever } j. \tag{2}$$

This leads to a set of linear inequalities defining the convex polyhedron V_i (which belongs to the class of simplicial complexes in the terminology of algebraic topology [34]) around each site $\mathbf{x}_i$:

$$\mathbf{x} \cdot (\mathbf{x}_j - \mathbf{x}_i) \leqslant \tfrac{1}{2}(\mathbf{x}_j + \mathbf{x}_i) \cdot (\mathbf{x}_j - \mathbf{x}_i). \tag{3}$$

Alternative constructive methods for any dimension are devised in [26–29]. We recall the definition of a simplex in dimension d: it is the convex hull of a set of $(d+1)$ points; it is nondegenerate when its volume is nonvanishing.

The dual Delaunay construction is a tiling of the space by simplices whose vertices are the original cluster points x_i, with the following property:

THEOREM 1. *A d-dimensional simplex $S_{i_1, i_2, ..., i_{d+1}}$ belongs to the Delaunay tesselation in a d-dimensional space if no further vertex but the generating ones fall into the d-dimensional circumsphere to the simplex.*

The simplex S is characterized uniquely by the set of indices of the vertex points $i_1, i_2, ..., i_{d+1}$. It is even possible to orient positively the simplices, by defining the ordered simplex $i_1 < i_2 < \cdots < i_{d+1}$ and all those related by an even permutation as positive; it is also possible to classify and order the simplices, with the preceding convention, into lexicographic order (which allows fast search and ordering). But we have developed a nonalgebraic version here.

The center of the circumscribing sphere of simplices in the d-dimensional space is a vertex point of the dual Voronoi graph, which corresponds to the center of a void between adjacent atoms. In the case of packing of spheres of unequal radii, it may

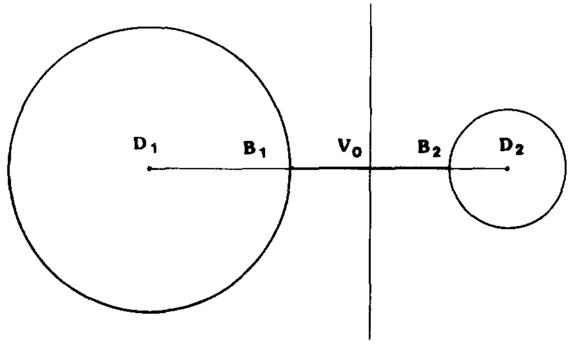

FIG. 1. In the case of two unequal balls (D_1 and D_2), the Voronoi plane may be defined as the bisecting plane of segments B_1B_2, instead D_1D_2 as in the usual case. This ensures that the Voronoi vertices are centered in the voids between the spheres.

be interesting to modify the definition of Voronoi cells in order to preserve this property: the boundary plane of the Voronoi cell bisects the segment outside the spheres joining the centers of two spheres (Fig. 1). In this way it coincides with the common tangent plane in the case of touching spheres; but the usefulness of the circumscribed sphere to a Delaunay simplex is then weakened, since the center of the sphere does no more coincide with the dual Voronoi vertex point. We present also in Section 3 an original application of the duality of honeycombs for a fast and straightforward construction of the full dual Voronoi tesselation by inspection only, once the Delaunay tiling is known.

3. A Global Construction of the Delaunay Tesselation

There exist already published algorithms in 2, 3, or higher dimensions for the construction of the Delaunay graphs [31–33].

First, we show how to build the smallest d-dimensional circumscribing sphere to a di-dimensional simplexe $(\mathbf{x}_0, ..., \mathbf{x}_{di})$. Let $\mathbf{c}$ denote its center, and r its radius. Then

$$r^2 = (\mathbf{c} - \mathbf{x}_0)^2 = (\mathbf{c} - \mathbf{x}_1)^2 = \cdots (\mathbf{c} - \mathbf{x}_i)^2 \cdots = (\mathbf{c} - \mathbf{x}_{di})^2 \tag{4}$$

has to be minimal. This is equivalent to the standard Lagrange problem:

$$r^2 = (\mathbf{c} - \mathbf{x}_0)^2 \qquad \text{minimal} \tag{5}$$

$$\text{subject to the di constraints:} \qquad (\mathbf{c} - \mathbf{x}_i)^2 = (\mathbf{c} - \mathbf{x}_0)^2, \qquad i = 1, di. \tag{6a}$$

The constraints are in fact linear forms in $\mathbf{c}$, which describe the bissecting planes to the segments $(\mathbf{x}_0, \mathbf{x}_i)$:

$$(\mathbf{x}_i - \mathbf{x}_0) \cdot (\mathbf{c} - \mathbf{x}_0) = \tfrac{1}{2}(\mathbf{x}_i - \mathbf{x}_0)^2. \tag{6b}$$

Thus, we obtain for the coordinates of the center **c** of the circumscribing sphere:

$$\mathbf{c} = \mathbf{x}_0 + \sum_{i=1}^{di} p_i(\mathbf{x}_i - \mathbf{x}_0). \tag{7a}$$

The set p_i is the solution of the linear system:

$$\sum_{j=1}^{di} (\mathbf{x}_i - \mathbf{x}_0) \cdot (\mathbf{x}_j - \mathbf{x}_0)\, p_j = \frac{1}{2} (\mathbf{x}_i - \mathbf{x}_j)^2, \qquad i = 1, di. \tag{7b}$$

We propose here a global construction, which is based on the recursive property of Theorem 1 which we extend in the following way:

THEOREM 2. *If no further point falls into the smallest d-dimensional circumsphere to a di-dimensional simplex* $(0 \leqslant di \leqslant d)$, *this simplex belongs to the Delaunay tiling.*

We illustrate this theorem on Fig. 2. The proof is: let b be the d-dim. circumsphere to such a di-dim. simplex S; then b is contained in the reunion of the intersections of b with the d-dim. circumspheres $\{B_l\}$ to the d-dim. Delaunay simplices containing S

$$b \subset \bigcup_l (b \cap B_l). \tag{8}$$

No points other than those generating S (thus b) are contained in any such intersection $b \cap B_l$, by definition of b.

We qualify as "normal" a tile satisfying Theorem 2. The vertices, which are Delaunay tiles of dimension 0 and the usual Delaunay tiles of maximal dimension d are normal. Indeed, there is a null sphere circumscribing each vertex, and Theorem 2 is equivalent to Theorem 1 for the maximal dimension d. The normality of Delaunay tiles of intermediate dimension $0 < di < d$ is only a sufficient condition (cf. Fig. 2).

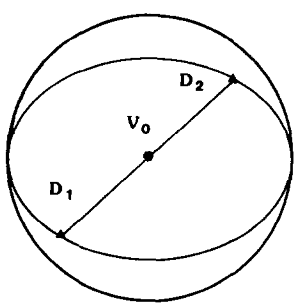

FIG. 2. An illustration of the theorem (9) for a 3-dimensional tesselation. The segment D_1D_2 is a 1-dim. Delaunay tile, which is part of the 3-dim. Delaunay tesselation, if no further Delaunay vertex falls within the 3-dim. circumspheres (centered at V_0) to D_1D_2.

In the following, we use two operations: the first, which we call P like "Pyramid" or "Primitive," allows to build a $(di+1)$ simplex by adjoining a further point to a d-dim. simplex, and by checking its normality; the second, B like "Boundary," is to build all $(di-1)$ simplices bounding the original di-dim. simplex. This is done by dropping out one index in the ordered list of the $(di+1)$ vertices generating the original simplex; we obtain $(di+1)$ such $(di-1)$-dim. tiles, corresponding to all the possible positions of the dropped index in the original list. All tiles obtained as a part of a normal tile must also be considered as valid Delaunay tiles, even though they are not normal.

We propose the following algorithm to build the whole Delaunay tesselation.

ALGORITHM 1.

(1) Initialize the ordered list of tiles by the original vertices; let all of them be unmarked.

(2) If no more unmarked tile is available, stop; else proceed.

(3) Select an unmarked tile t; mark it; let its dimension be di;

- (3.1) Revise the list of tiles by new normal $(di+1)$-dim. tiles built from t by operation P; let them be unmarked.
- (3.2) Revise the list of tiles by the new $(di-1)$-dim. tiles not yet in the list, obtained from t by operation B; let them be unmarked.

(4) Repeat from (2).

We prove the validity and the performances of this algorithm, by comparing it to that of Ogawa *et al.* [33].

First, there exists at least one d-dim. Delaunay tile for each vertex which may be built by repeated primitive operation P upon it [33]. Here, we need only one for the whole tesselation. Second, all Delaunay tiles will be obtained, since the d-dim. tiles will be exhausted by repeated operations of B and P on the unmarked d-dim. tiles already in the list. For a $(d-1)$-dim. tile "all" in step 3.2 reduces to "one, if any." All other tiles may be obtained by the operation of Boundary, if not obtained earlier. This is realized naturally, just by selecting the last unmarked tile in step 2. The lexicographic order is useful in several aspects: it allows fast search for the existence of a tile and it also allows updating the list with new tiles, the order being conserved. Moreover, it provides a natural labelling for the tiles:

DEFINITION 1. The dimension di of a tile and its index i among the di-dim. tiles entirely characterizes a tile, which we designate as $(di : i)$.

Once the families of Delaunay simplices are completed, it is possible to build trees, which denote the parentship between simplices of adjacent dimension,

$$(di+1 : j) \text{ is a child of } (di : i) \text{ if it contains } (di : i). \tag{9}$$

(resp.

$$(di-1 : j) \text{ is a parent of } (di : i) \text{ if it is contained in } (di : i)). \tag{10}$$

It is only necessary to build the tree of children, the tree of parents merely being the inverse tree of the latter. This tree of children is equivalent to the Bettis's incidence coefficients, when brought into algebraic form [34] or to the incidence matrices defined by Coxeter [15]. Such a tree provides the full information on the Delaunay graph of simplices; for instance, all neighbors of a site i are the set of children $\{(1:j)\}$ of $(0:i)$. But from a closer examination of this tree, we learn that we also have full information about the dual Voronoi construction. We note $(di:i)^*$ is a dual Voronoi tile (a general convex polytope). The element $(0:i)^*$ is known: it is the center of the circumscribing sphere to the simplex $(d:i)$.

More generally, the correspondence is

$$(di:i) \underset{*}{\longleftrightarrow} (d-di:i)^* \tag{11}$$

and vectors belonging to conjugate sets are orthogonal.

For instance, the usual description of the Voronoi cell V_i relative to the atom i $(0:i)$ is to build the convex hull of the points obtained by applying the duality transformation to the last generation of the children of $(0:i)$.

We show now that is possible to make precise all intermediate dual elements, and to give a complete description of each tile $(di:i)^*$ in terms of its boundary. Let us suppose that all $(dj:j)^*$ are known, for $dj<di$; then $(di:i)^*$ is the convex polytop, the boundary of which are cycles of the form

$$(di:i)^* = ((di-1:j_1)^*, ..., (di-1:j_i)^*). \tag{12}$$

The set $j_1 \cdots j_i$ is determined in the following way:

take the dual of $(di:i)^* \to (d-di:i)$

take its children $(d-di+1:j_1), ..., (d-di+1:j_i)$

transform back by duality.

This is a recursive proof for obtaining all Voronoi tiles $(di:i)^*$; we converted it into an iterative algorithm by iterating over the dimension di^* from 0 to d.

The scheme we propose is very economical for a global Delaunay and Voronoi construction and is valid independently of the dimension and the imbedding manifold. In the case of Delaunay–Voronoi construction on infinite manifolds, or manifolds with boundaries, the preceding description may be completed for the irregular "outer cells" $(1:i)^*$: if $(d-1:i)$ has only one son, say $(d:j)$ instead of two, a ghost son, mirror point of $(0:j)^*$ with respect to the plane defined by $(d-1:i)$, may be introduced in order to define unambiguously (11). Another way we use here, is to state that $(1:i)^*$ is a half-line starting from $(0:j)^*$, orthogonal to $(d-1:i)$. We retained this last solution.

In the next section, we discus the algorithm on an example, and also its performance and improvements.

3. Numerical Implementation and Example

We implemented the preceding algorithm in APL, in about one hundred statements, in a form easily convertible into a more efficient language at execution time (FORTRAN, even on a vector computer). The trees (Delaunay simplices, children, Voronoi tesselation) are implemented as vectors, with one or two levels of pointers. For each dimension di, the lexicographic order is maintained on the Delaunay tiles in order to allow fast search. We illustrate the algorithm on an example, which may be checked by hand. We apply the tesselation creation to a set of five points in the Euclidian plane; the coordinates are given in Table I.

In Table II, we indicate in the third column the family of Delaunay simplices obtained at the end of the first phase, as the ordered list of the indices of its vertices. The Voronoi vertices which are obtained simultaneously as the centers of the circumscribing spheres to the d-dim. Delaunay simplices are reported in column 3. In column 4 of Table II, we report the children of $(di : i)$. In the last column appear the Voronoi tiles, which, according to the prescription (12), are built upwards. We use a simplified notation $[\cdots]$ instead of $(:)^*$ in this table, omitting even 0: .

We show the corresponding results on Fig. 3. Namely there appear irregular edges obtained only in the downwards Boundary operation of the Delaunay tesselation. We mention also that the subsets of a regular Voronoi tile are cycles ($BB\ (di : i)^* = 0 \bmod 2$), and that the cells on the boundary are very naturally described. We did not discuss here the case of degeneracy, since this has been widely done by others.

The structure of the algorithm given in the preceding section is simple and flexible. It exhibits clearly the parentship of tiles of the whole tesselation. Even in this form, its performances are very different, depending on which side of the list one selects the unmarked tiles to be processed. Indeed, contrary to the Boundary operation which is straightforward, the Primitive operation is more costly. Let n be the number of initial points; the implementation of Theorem 2 requires n d-dim. spheres determination (a linear system of rank d) and n distance comparisons for each sphere, in order to build all normal adjacent $(di+1)$-dim. tiles to a di-dim. one. In fact, if one requires only one new normal $(di+1)$-dim. tile, an alternative Primitive procedure $P1$ may be used, the cost of which is the construction of only n spheres [33].

TABLE I

Set of Delaunay Vertices

Designations	Coordinates
(0) (0 : 0)	0.55, 0.6
(1) (0 : 1)	0.1, 0.3
(2) (0 : 2)	0.4, 0.85
(3) (0 : 3)	0.7, 0.9
(4) (0 : 4)	0.9, 0.3

TABLE II

An Example

Dim	Index	Delaunay simplices	Children	Voronoi tiles	di*
0	(0)	(0)	(1 : 0, 1, 2, 3)	[[[0][1]][[0][2]][[2][3]][[1][3]]]	2
	(1)	(1)	(1 : 0, 4, 5)	[[[0][1]][[0](1 : 4)][[1](1 : 5)]]	
	(2)	(2)	(1 : 1, 4, 6)	[[[0][2]][[0](1 : 4)][[2](1 : 6)]]	
	(3)	(3)	(1 : 2, 6, 7)	[[[2][3]][[2](1 : 6)][[3](1 : 7)]]	
	(4)	(4)	(1 : 3, 5, 7)	[[[1][3]][[1](1 : 5)][[3](1 : 7)]]	
1	(0)	(0 1)	(20)	[[0][1]]	1
	(1)	(0 2)	(20)	[[0][2]]	
	(2)	(0 3)	(2 : 1, 2)	[[2][3]]	
	(3)	(0 4)	(2 : 1, 3)	[[1][3]]	
	(4)	(1 2)	(2 : 2, 3)	[[0](1 : 4)]	
	(5)	(1 4)	(2 : 1)	[[1](1 : 5)]	
	(6)	(2 3)	(2 : 2)	[[2](1 : 6)]	
	(7)	(3 4)	(2 : 0, 3)	[[3](1 : 7)]	
2	(0)	(0 1 2)	(null)	[0]	0
	(1)	(0 1 4)	(null)	[1]	
	(2)	(0 2 3)	(null)	[2]	
	(3)	(0 3 4)	(null)	[3]	

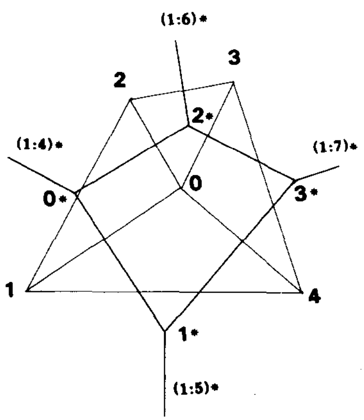

FIG. 3. Graphical representation of the two dual tesselations of the example: thin line (Delaunay); thick line (Voronoi). Note the anomalous 1-dim. tiles (1 4)(3 4)(1 2).

DEFINITION 2. *Primitive* 1. Let t a di-dim. tile be given; then the $(di+1)$-dim. tile $t \cup \mathbf{x}_j$ with minimal circumradius is a new normal tile.

If one builds the Delaunay tesselation by selecting the unmarked tiles on the left (lower dimension) of the list of tiles being created. Primitive operations of general type are mainly required, and the cost of the algorithm would be $O(n^3)$ at least. By selecting the unmarked tiles on the right (the unmarked simplices existing in the list of highest dimension), one builds as fast as possible a first-dimensional Delaunay tile. The procedure Primitive 1 just discussed may be used as an alternative to our more general (and costly) primitive. One exhausts then the d-dimensional Delaunay tiles, with repeated operations of Boundary and Primitive. Here again, a second procedure for Primitive of Ogawa *et al.* may be used (of order n), instead our more general (but costly) one:

DEFINITION 3. *Primitive* 2. For a $(d-1)$-dimensional tile t, parent of an existing (d-dimensional) tile, find the vertex x_j (if any) in the half-space delimited by the plane containing t, opposite to the existing child, such that the sphere circumscribed to $(\mathbf{x}_j \cup t)$ has the minimal radius.

Once the d-dim. tiles are exhausted, it is possible to complete the tree of tiles downwards over dimension by the fast Boundary operation. In this way, the Delaunay tesselation realization becomes a frontal growth process. It seems to be of order n^2, namely n Primitive 2 operations. In fact, it can be reduced further to order n by restricting the sites to be considered in the primitive process to a neighborhood of the tile t defined by the usual metric distance [26, 33]. For this purpose, we also propose a conjecture similar to Euler's theorem, which allows checking if the environment of a tile is completed.

Conjecture 1. Let n_p be the number of tiles of dim. p, children of a given tile $(di:i)$. Then

$$I((di:i)) = (-1)^d \sum_{p=di}^{d} (-1)^p n_p \tag{13}$$

is an indicatrix of completeness of environment, valued to 0 for incomplete embedding, to 1 for full embedding.

TABLE III

Voronoi Vertices

Designation	Coordinates	Radius
[0](0 : 0)*	−0.237, 0.5820	0.313
[1](0 : 1)*	−0.5, 0.416	0.416
[2](0 : 2)*	−0.566, 0.7800	0.180
[3](0 : 3)*	−0.875, 0.6250	0.325

The reader may check the plausibility of our conjecture on examples. Table II and Fig. 3 may be used. With the last refinement, the full explicitation of the tree of children becomes necessary, and it must be built simultaneously to the Delaunay tesselation. This would allow taking into account the full information about the Delaunay tesselation at its actual stage of formation, and also avoiding any useless primitive operation.

4. Conclusion

In this paper, we collected and discovered (merely rediscovered) a lot of fundamental results which allowed us to gain a better insight into the structure of the dual Delaunay and Voronoi tesselations. Contrary to other efficient methods for constructing the Delaunay tesselation, where the points are added one by one and the sets revised, like [29, 35, 36], the one presented here is global, independent of the dimension of the space, and conceptually very simple. The algorithm proposed is able to be vectorized. It also realizes an illustration of algebraic topology (duality mainly), since it possesses a natural orientation convention defined in the text after Theorem 1. The new results are mainly the definition of normal tiles, which uses the smallest d-dimensional sphere circumscribing a di-dimensional simplex, and an original application of the duality, which allows a full description of any Voronoi or Delaunay tile in terms of its boundary tiles. Note also that the duality is symmetric; i.e., it may be used in the reverse way. Our conjecture about the completeness of a neighborhood seems also an interesting property.

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