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A New Algorithm for Three-Dimensional Voronoi Tessellation

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A new efficient algorithm for computing the Voronoi tessellation in three dimensions is presented. The Voronoi tessellation is obtained by constructing Delaunay tetrahedra. The complete set of these tetrahedra corresponds to that of a single Voronoi polyhedron.

1. INTRODUCTION

The need for constructing the Voronoi tessellation has increased recently, mainly for the purpose of describing, analyzing, and modelling the spatial patterns of points (atoms, animals, houses, cities, stars, and so on) [1]. Accordingly, an efficient algorithm is required for computing the Voronoi tessellation of a given set of points (hereafter, we use the term "atom" in place of "point" to avoid confusion). Although many authors might have an implicitly devised method for constructing Voronoi polygons or Voronoi polyhedra, it seems that the algorithms which have been explicitly published so far are rather few. As far as we know, the only published algorithms are by Green and Sibson [2] for Voronoi polygons and by Brostow, Dussault, and Fox [3] and Finney [4] for Voronoi polyhedra. Recently, Bowyer [5] and Watson [6] presented algorithms for computing k-dimensional Voronoi tessellations ($k = 2, 3, 4, \ldots$). The purpose of this paper is to give a new efficient method of Voronoi tessellation in three-dimensional space, which uses a different

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algorithm from those mentioned above (Tanemura, Hiwatari, Matsuda, Ogawa, Ogita, and Ueda [7]).

In Section 2, some definitions are given. In Section 3, the main part of the algorithm is outlined. Section 4 elucidates in detail one of the steps of the algorithm. Proofs of theorems are given in Section 5. In Section 6, some technical details of programming the algorithm are presented. In Section 7, efficiency of the algorithm and comparisons with other algorithms are given. Finally, Section 8 gives some possible improvements and a generalization.

2. Some Definitions

Let N atoms be distributed in a box V of finite size. In the following, we assume that this box is a cube of side length L ($|V| = L^3$). Assume that the whole three-dimensional space is covered, without any gap or any overlap, by replicas of this box so that each atom in the original box V is periodically located in each of three directions outside the box with period L.

Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ be the coordinates of atoms in the original box. Denote all of the periodic images of each $\mathbf{x}_i$ representatively by $\mathbf{X}_i$ ($i = 1, \ldots, N$). Then, the *Voronoi region* Π_i of atom i inside V is defined by the following set of points $\mathbf{x}$ of the space:

$$\Pi_i = \{\mathbf{x} \mid d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{x}_j) \text{ and } d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{X}_k), \text{ for all } j \neq i \text{ and for all } k, \text{ respectively}\}, \tag{1}$$

where $d(\mathbf{x}, \mathbf{y})$ is the Euclidean distance between $\mathbf{x}$ and $\mathbf{y}$. In other words, Π_i is the set of points which is nearer to $\mathbf{x}_i$ than any other $\mathbf{x}_j$'s and $\mathbf{X}_k$'s. Note that each region Π_i is the intersection of the open half-spaces bounded by the perpendicular bisectors of the segments joining $\mathbf{x}_i$ with each of the other $\mathbf{x}_j$'s and $\mathbf{X}_k$'s. Hence, Voronoi regions are convex polyhedra with finite size according to definition (1). Each Π_i is called a *Voronoi polyhedron*. This is a generalized concept of a Wigner–Seitz cell which is assigned to each atom in a regular lattice and which is principally used in solid state physics.

The above definition (1) of a Voronoi polyhedron is slightly different from that of Rogers [8] because the periodic boundary conditions are imposed in our formulation. The set of Π_i's ($i = 1, \ldots, N$) and its periodic repetitions constitute a tessellation of space, i.e., a *Voronoi tessellation*, which is unique for a given configuration of atoms inside V.

A pair of atoms i and j whose Voronoi polyhedra Π_i and Π_j have a face in common is called a *contiguous pair* and a member of the pair is said to be *contiguous* to the other member. By joining all of the contiguous pairs of atoms, we obtain a network. In this network, a set of four atoms which are contiguous with one another forms a tetrahedron. The set of tetrahedra constructed in such a manner constitutes a new tessellation, which is called the *Delaunay tessellation*. These two tessellations, Voronoi and Delaunay, are dual to each other. We call the tetrahedron in the

Delaunay tessellation the *Delaunay tetrahedron* and often abbreviate it as DT. For each DT, let us describe a circumsphere, i.e., a circumscribing sphere.

Remark 1. The circumcenter, i.e., the center of the circumsphere, of a DT is a vertex of the Voronoi tessellation.

From the definition of the Voronoi tessellation, the four atoms which form the DT are equidistant from the vertex concerned, and thus Remark 1 follows.

Remark 2 (Contiguity Condition). The circumsphere of a DT is *empty*, that is, there is no atom inside this sphere.

If the fifth atom exists inside the sphere, it is nearer to the circumcenter than the four atoms on the surface of the sphere. Therefore, the center cannot be the common vertex of the Voronoi polyhedra of the four atoms. Thus, Remark 1 leads to Remark 2.

At a vertex of the Voronoi tessellation, generally, four polyhedra meet. However, if a vertex happens to have five or more polyhedra in common, the vertex is said to be *degenerate*. Obvious degenerate cases can be found for typical crystalline lattice structures. Although the algorithm presented in this paper works for both degenerate and nondegenerate cases, we assume here the degeneracy is absent in the configurations with which we are concerned. This point will be discussed in Section 6.

Finally, let us introduce a symbol $\{i, j, k, \ldots\}$ in order to indicate a set of atoms $i, j, k, \ldots$, and geometrical objects formed by these atoms. For example, the symbol $\{i, j\}$ represents the pair of atoms i and j, the segment which joins i and j, and the line which passes through i and j. The symbol $\{i, j, k\}$ indicates the set of three atoms i, j, and k, the triangle which is obtained by connecting i, j, and k by segments, the face surrounded by this triangle, and the plane which contains this face. The meaning of the symbol will be indicated on each occasion by putting a term in front of the symbol.

3. Algorithm

The main part of our algorithm for computing the Voronoi tessellation is composed of the procedure for constructing a single Voronoi polyhedron. Voronoi tessellation is obtained by the repeated use of this procedure for all of the atoms $i = 1, \ldots, N$. Our procedure of constructing Π_i, i.e., Voronoi polyhedron of atom i, consists essentially of obtaining all DT's each of which has the atom i as a common vertex. Denote such a set of DT's by T_i and call it the complete set of DT's for atom i. From the arguments in Section 2, obtaining T_i is equivalent to obtaining Π_i. Note that T_i constitutes a polyhedron, not necessarily convex, whose vertices are atoms. It will be referred to as a *contiguity polyhedron* of atom i. Let C_i be a set of such vertex atoms of the polyhedron. Each member of C_i corresponds to a face of Π_i, the face being the perpendicular bisector of that member of C_i and the atom i. The face of Π_i which corresponds to a certain atom, say j, can be determined by DT's of T_i which

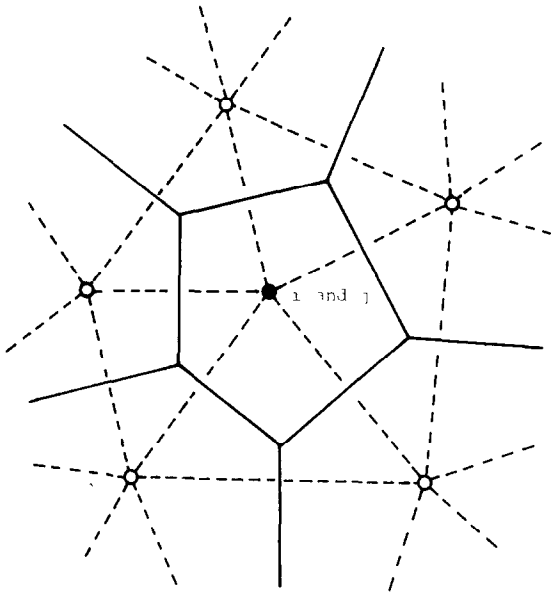

FIG. 1. Topological illustration of a portion of Π_i. The atom j which is contiguous to the central atom i is represented by a closed circle. The circle also represents the contiguous pair $\{i,j\}$. The polygon in the central part indicates the face which is produced by the pair $\{i,j\}$. Open circles are the atoms which are contiguous to both atoms i and j. Dotted triangles represent DT's.

have the atoms i and j as common vertices. Figure 1 is a two-dimensional representation of a three-dimensional structure. Note that the atom j is "above" the atom i (out of the page). The vertices of Π_i are the circumcenters of the respective member of T_i. As can be seen from Fig. 1, other geometries of Π_i, edges for instance, also can be determined from the connectivity among the elements of T_i. Therefore, the efficiency of the algorithm depends on how quickly we can search T_i and the connectivity in T_i.

Let S_i be a set of atoms surrounding atom i and let us assume S_i includes C_i, i.e., $S_i \supset C_i$. Note that S_i does not include the atom i itself. Under the assumption that S_i is already known (the method of determining S_i will be given in Section 6), our task is to find the contiguous set of atoms C_i from the set S_i. The algorithm for obtaining Π_i follows.

Step 1. Find the atom i_1 which is nearest to the atom i. Then i_1 is contiguous to i (Theorem 1) and is a member of C_i. Set $C_i \leftarrow i_1$.

Step 2. Consider a set of triplets $\{i, i_1, j\}$, where $j \in S_i$ and $j \neq i_1$. Find the atom $j = i_2$ so that the triangle $\{i, i_1, i_2\}$ has the minimum circumradius, i.e., the radius of the circumscribing circle of the triangle, in the set of triangles considered above. Then the triangle $\{i, i_1, i_2\}$ constitutes one of the faces of a DT (Theorem 2). Set $C_i \leftarrow i_2 \cup C_i$.

Step 3. Consider a set of quartettes $\{i, i_1, i_2, j\}$, where $j \in S_i$ and $j \neq i_1, i_2$. Find the atom $j = i_3$ so that the tetrahedron $\{i, i_1, i_2, i_3\}$ has the minimum circumradius, i.e., the radius of the circumscribing sphere of the tetrahedron, in the set of tetrahedra considered above. Then the tetrahedron $\{i, i_1, i_2, i_3\}$ is a DT (Theorem 3) and is a member of T_i. This tetrahedron is called an initial DT. Set $T_i \leftarrow \text{DT}\ \{i, i_1, i_2, i_3\}$ and $C_i \leftarrow i_3 \cup C_i$.

Step 4. Construct the complete set of DT's, T_i, starting from the initial DT obtained in steps 1–3. We shall explain this step in detail in the next section.

Step 5. Evaluate geometrical quantities of Π_i, i.e., volume, surface area, etc.

Repeat steps 1–5 for all atoms $i = 1, \ldots, N$; then the Voronoi tessellation is complete. Proofs of the theorems referred to here will be given in a later section.

4. Details of Step 4

In Step 4 of the algorithm, the DT's of T_i are detected one after another by the elementary procedure which will be given below. The procedure utilizes the information about a certain DT of T_i obtained earlier, starting with the initial DT defined in Section 3. For each member i_α of C_i, the detection of DT's is continued until DT's enclose the contiguous pair $\{i, i_\alpha\}$ without any gap. Step 4 ends when the DT's connect all of the contiguous pairs $\{i, i_\alpha\}$, $i_\alpha \in C_i$.

Elementary Process of Detecting a New DT

Suppose a DT $\{i, i_\alpha, i_\beta, i_\gamma\}$ is known as a member of T_i. Then, through the knowledge of this DT, we can obtain a new DT $\{i, i_\alpha, i_\beta, i_\delta\}$ such that these two DT's have the triangular face $\{i, i_\alpha, i_\beta\}$ in common (see Fig. 2).

Remark 3. The atoms i_γ and i_δ are located on opposite sides of the plane $\{i, i_\alpha, i_\beta\}$.

Denote by $H_i(\alpha\beta \mid \gamma)$ the half-space which is determined by the plane $\{i, i_\alpha, i_\beta\}$ and which does not contain i_γ. Further denote by $S_i(\alpha\beta \mid \gamma)$ the subset of S_i which is inside the half-space $H_i(\alpha\beta \mid \gamma)$. Then (from Remark 3) the fourth vertex atom i_δ of the new DT is found from the set $S_i(\alpha\beta \mid \gamma)$.

In order to find i_δ just mentioned, we surround each atom j of $S_i(\alpha\beta \mid \gamma)$ with a sphere which circumscribes the atom j itself and the triplet $\{i, i_\alpha, i_\beta\}$. Then the atoms of $S_i(\alpha\beta \mid \gamma)$ are characterized by only one parameter. To see this, take the X and Y axes arbitrarily in the plane $\{i, i_\alpha, i_\beta\}$ and take as the positive direction of the Z axis the normal of this plane to the side of $H_i(\alpha\beta \mid \gamma)$. The Z-coordinate value of the center of the sphere attached to the atom j, as defined above, represents the position of atom j relative to the triplet $\{i, i_\alpha, i_\beta\}$.

From the above discussion and from the contiguity condition (see Remark 2), the fourth vertex atom i_δ of a new DT which we are seeking will have the smallest Z

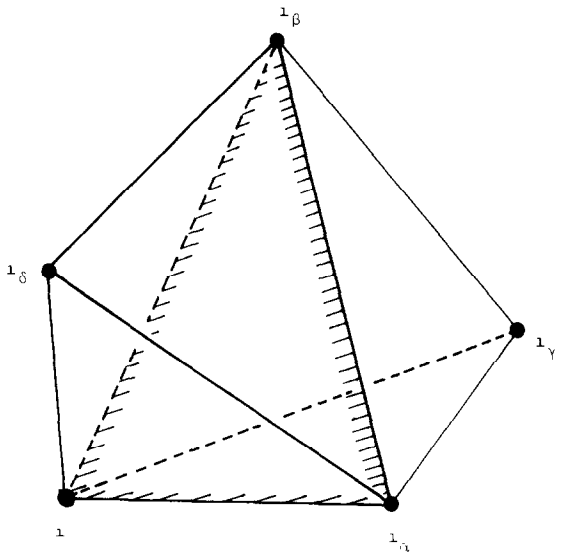

FIG. 2. Two DT's which have the triangular face $\{i, i_\alpha, i_\beta\}$ in common.

value of the *sphere center* (not of the atom) among the atoms of $S_i(\alpha\beta \mid \gamma)$ (Theorem 4). Figure 3 illustrates this circumstance.

Thus, the elementary process of detecting a new DT is elucidated. Each time a new DT is obtained, it is added to the list of T_i. As regards the fourth vertex atom of the new DT, it should be searched for in the list of C_i so far obtained and should be added to that list only if it is not yet contained in C_i.

Closing of DT's *around a Contiguous Pair* $\{i, i_\alpha\}$

According to the procedure described above, we detect DT's sequentially in such a way that they have a contiguous pair $\{i, i_\alpha\}$ in common until the DT's enclose the pair $\{i, i_\alpha\}$ without any gap, where i_α is any member in the list C_i so far obtained. Assume that a certain number of DT's is already found around the pair $\{i, i_\alpha\}$ and that the pair is not yet enclosed by DT's (Fig. 4). Each triangle in Fig. 4 represents each DT which has the pair $\{i, i_\alpha\}$ as a common edge. The pair is represented by a point in this figure as in Fig. 1. To indicate whether or not DT's are constructed on both sides of a triangular face which meets the pair $\{i, i_\alpha\}$ or, equivalently, whether the relevant face is completed or not, we assign to each face, $\{i, i_\alpha, i_\beta\}$ say, a count index $l_{\alpha\beta}$. The index represents the number of constructed DT's which have a relevant face in common. Therefore, if $l_{\alpha\beta} = 2$, the DT's are constructed on both sides of the face $\{i, i_\alpha, i_\beta\}$ and at that time the face is completed. In Fig. 4, for example, $l_{\alpha\beta} = 1$, $l_{\alpha\gamma} = 2$, and $l_{\beta\gamma} = 1$. Initially, each of the count indices is set to zero. At every stage of detecting a new DT, the count indices of relevant faces should be renewed. As an example, in Fig. 4, a new DT which is about to be detected is indicated by a triangle with dotted lines. When this DT is detected, i_δ being its fourth vertex, count indices

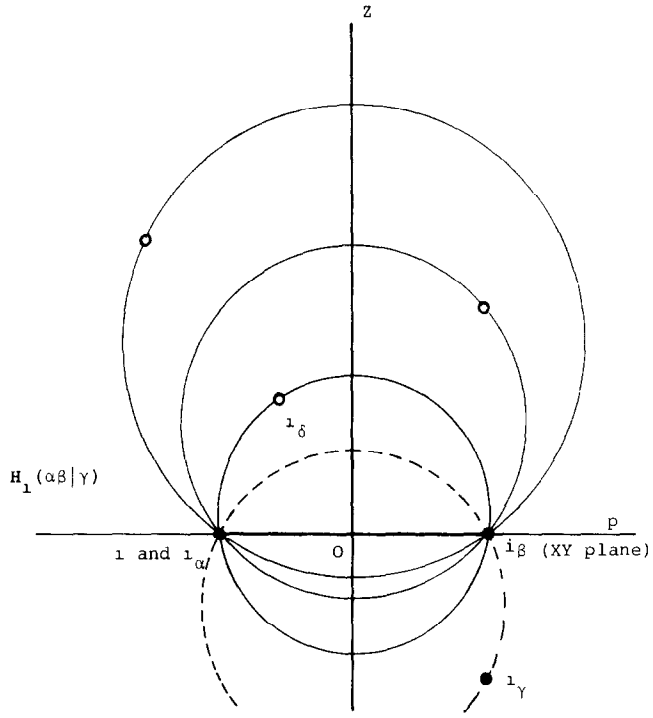

FIG. 3. Schematic diagram to show the elementary process of detecting a new DT. Horizontal line p in the figure indicates the XY plane. Two closed small circles on the line p represent atoms i_α and i_β. One of them should be thought to indicate the atom i itself. The closed small circle below the line p is the atom i_γ. Dashed circle corresponds to the circumsphere of DT $\{i, i_\alpha, i_\beta, i_\gamma\}$. Open half-plane above the line p corresponds to $H_i(\alpha\beta \mid \gamma)$. Open small circles are the element atoms of $S_i(\alpha\beta \mid \gamma)$. Solid circles correspond to spheres which are attached to these atoms. In the figure, atom i_δ is a vertex of the new DT.

$l_{\alpha\beta}$, $l_{\alpha\delta}$, and $l_{\beta\delta}$ should be increased by one. If all of the count indices $\{l_{\alpha\cdot}\}$ of respective faces which meet the pair $\{i, i_\alpha\}$ have the value 2, then the DT's close the pair without any gap. At that time, an index m_α, which is attached to the atom i_α, is set equal to unity and the atom i_α can be removed from the set S_i because i_α never appears again as a vertex of another DT.

Closing of DT's *around the Central Atom i*

Applying the above procedures, we continue the detection of DT's until $m_\alpha = 1$ is attained for all of the pairs $\{i, i_\alpha\}$, $i_\alpha \in C_i$. By examining the list of C_i exhaustively, it can be determined when the set of detected DT's, T_i, encloses the atom i without any gap, or when the construction of Π_i is achieved. This is the stopping rule of step 4.

As a summary of this section, let us itemize the substance of step 4 as follows:

4.0. Clear $\{m_\alpha\}$ and $\{l_{\alpha\beta}\}$.

4.1. Set $\alpha \leftarrow 1$.

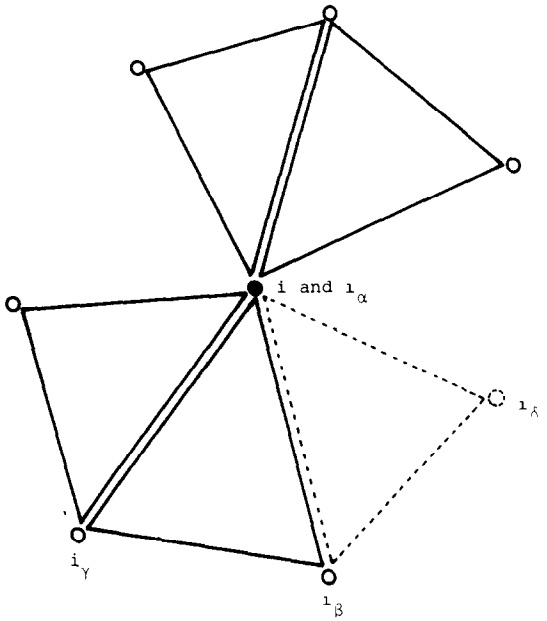

FIG. 4. Schematic diagram of successive construction of DT's. The closed circle represents the contiguous pair $\{i, i_\alpha\}$. This figure indicates the halfway stage of closing DT's around the pair $\{i, i_\alpha\}$. For details, see text.

4.2. Pick out i_α from C_i. If the list of C_i is exhausted, go to step 5; otherwise go to step 4.3.

4.3. If $m_\alpha = 1$, set $\alpha \leftarrow \alpha + 1$ and go to step 4.2; otherwise go to step 4.4.

4.4. Find, in the list T_i of existing DT's, a DT $\{i, i_\alpha, i_\beta, i_\gamma\}$ which has the edge $\{i, i_\alpha\}$ in common and for which $l_{\alpha\beta} = 1$.

4.5. Set $S_i(\alpha\beta \mid \gamma) \leftarrow S_i \cap H_i(\alpha\beta \mid \gamma)$ and describe a circumsphere to each quartette $\{i, i_\alpha, i_\beta, j\}$, $j \in S_i(\alpha\beta \mid \gamma)$ and $m_j \neq 1$.

4.6. Set $i_\delta \leftarrow j_{\min}$ for which the center of the circumsphere of the tetrahedron $\{i, i_\alpha, i_\beta, j_{\min}\}$ has the minimum Z-coordinate value, including its sign, among the circumspheres obtained in step 4.5. X and Y axes are taken arbitrarily in the plane $\{i, i_\alpha, i_\beta\}$ and the Z axis is defined as the normal of this plane to the side of half-space $H_i(\alpha\beta \mid \gamma)$.

4.7. Set $T_i \leftarrow \text{DT}\ \{i, i_\alpha, i_\beta, i_\delta\} \cup T_i$. If $i_\delta \notin C_i$, set $C_i \leftarrow i_\delta \cup C_i$. Set $l_{\alpha\beta} \leftarrow l_{\alpha\beta} + 1$, $l_{\alpha\delta} \leftarrow l_{\alpha\delta} + 1$, and $l_{\beta\delta} \leftarrow l_{\beta\delta} + 1$. Set also $l_{\beta\alpha} \leftarrow l_{\alpha\beta}$, $l_{\delta\alpha} \leftarrow l_{\alpha\delta}$, and $l_{\delta\beta} \leftarrow l_{\beta\delta}$.

4.8. If all $\{l_{\alpha\cdot}\}$ are equal to 2, set $m_\alpha \leftarrow 1$. If all $\{l_{\beta\cdot}\}$ and/or $\{l_{\delta\cdot}\}$ are equal to 2, set $m_\beta \leftarrow 1$ and/or $m_\delta \leftarrow 1$. Then, go to step 4.3.

Note that at the stage just before step 5 is entered, the sets T_i and C_i are completely obtained and that, therefore, Π_i is constructed.

5. Proof of the Theorems

In this section, we present a proof of the theorems which are used in Sections 3 and 4 and which are the basis of the present algorithm. We first state Theorems 1–4 explicitly:

THEOREM 1. *Let an atom i_1 be the nearest to an atom i. Then, i_1 and i are contiguous with each other.*

THEOREM 2. *Consider a set of triangles $\{i, i_1, j\}$, $j \in S_i$ and $j \neq i_1$. Among them, suppose a triangle $\{i, i_1, i_2\}$ has the minimum circumradius. Then, the triangle is a face of a certain* DT, *that is, the three atoms i, i_1, and i_2 are mutually contiguous.*

THEOREM 3. *Consider a set of tetrahedra $\{i, i_1, i_2, j\}$, where $j \in S_i$ and $j \neq i_1, i_2$. Among them, suppose a tetrahedron $\{i, i_1, i_2, i_3\}$ has the minimum circumradius. Then, the tetrahedron is a* DT, *that is, the four atoms i, i_1, i_2, and i_3 are mutually contiguous.*

THEOREM 4. *Let a* DT $\{i, i_\alpha, i_\beta, i_\gamma\}$ *be an element of T_i. Consider a set of tetrahedra $\{i, i_\alpha, i_\beta, j\}$, where $j \in S_i(\alpha\beta \mid \gamma)$. Among them, suppose the circumcenter of a tetrahedron $\{i, i_\alpha, i_\beta, i_\delta\}$ has the minimum Z-coordinate value, where the coordinate Z of the circumcenter is defined as its distance to the plane $\{i, i_\alpha, i_\beta\}$ and the sign of the coordinate is chosen so that the coordinate of i_γ is negative. Then, the tetrahedron is a* DT, *that is, the four atoms i, i_α, i_β, and i_δ are mutually contiguous.*

[redacted] Lemmas 1–3 as a preliminary:

LEMMA 1. *Let a point A be on a sphere O and a point B be outside O. Then the center of the sphere O and its neighbourhood are on the same side as A with respect to the perpendicular bisecting plane of the segment AB* (Fig. 5).

Proof of Lemma 1. Generally a perpendicular bisector of a segment AB divides the whole space into two half-spaces; $PA > PB$ holds for any point P in one of them and $PA < PB$ for a point P in the other. Lemma 1 follows from the relation $OA < OB$ and from the fact that the point O is never on the bisecting plane. Q.E.D.

LEMMA 2. *Let C be the intersection circle of two spheres O and O'. Take a point P outside O and inside O'. Let O'' be the sphere passing through P and the circle C. Then the center O'' lies on the segment OO'.*

Proof of Lemma 2. It is evident that the center O'' lies on the line OO'. Consider the plane containing three points O, O', and P (Fig. 6). The circles O, O', and O'' are defined as the great circles of the corresponding spheres in the plane. Let A and B be

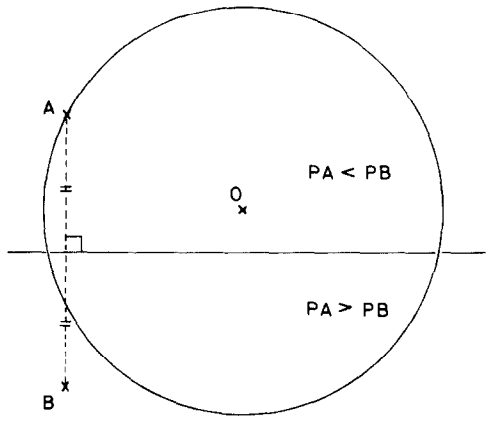

FIG. 5. See Lemma 1.

two intersections of the three circles. The segment AB is a diameter of the circle C. For each of the three circles O, O', and O'', an arc AB is defined as the part of the circle in the half-plane which is determined by the line AB and does not contain P. Let Q and Q' be the intersections of the line AP with the circles O and O', respectively. From the condition for the position of P, it follows that

$$\angle AQ'B < \angle APB < \angle AQB.$$

Then, from the relation between angles at the center and the circumference of a circle standing on the same arc AB defined above

$$\angle AO'B = 2\angle AQ'B, \qquad \angle AO''B = 2\angle APB, \qquad \text{and} \qquad \angle AOB = 2\angle AQB,$$

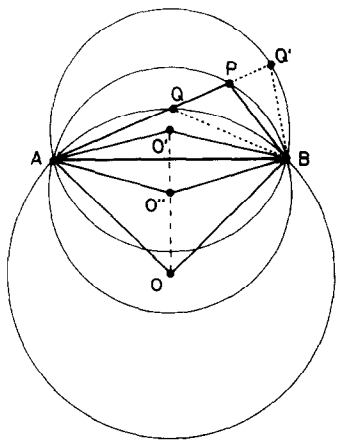

FIG. 6. See proof of Lemma 2.

and it follows that

$$\angle AO'B < \angle AO''B < \angle AOB.$$

Therefore O'' lies between O and O'. Q.E.D.

LEMMA 3. *The intersection of two spheres O and O' is a great circle C of the sphere O. Take a point P outside O and inside O'. Let O'' be the sphere passing through P and the circle C. Then the radius of O'' is smaller than that of O'* (Fig. 7).

Proof of Lemma 3. The situation is the special case of that in Lemma 2 where the center of O lies in the plane containing C. Then $\angle AO'B < \angle AO''B < \angle AOB = 2\angle R$ holds. By comparing two isosceles triangles $O'AB$ and $O''AB$, it is concluded that $AO'' < AO'$. Q.E.D.

On the basis of Lemmas 1–3, we can proceed to the proofs of Theorems 1–4.

Proof of Theorem 1. Let O_1 be the sphere whose diameter is the segment $\{i, i_1\}$. If atom j were inside O_1, j would be nearer to i than i_1. Therefore O_1 is empty. Lemma 1 says that the center O_1 and its neighbourhood are never nearer to an atom outside O_1 than to any of i and i_1. Then the perpendicular bisector plane $\{i, i_1\}$ separates the neighbourhood of O_1 into two Voronoi regions of i and i_1. Therefore these two atoms are mutually contiguous. Q.E.D.

Proof of Theorem 2. Let C be the circumcircle of the triangle $\{i, i_1, i_2\}$. Let O_2 be the sphere of which C is a great circle. The two spheres O_1 and O_2 intersect each other. As shown in the proof of Theorem 1, O_1 is empty. If atom j were outside O_1 and inside O_2, the circumradius of the triangle $\{i, i_1, j\}$ would be smaller than that of $\{i, i_1, i_2\}$ according to Lemma 3. This contradicts the condition. Therefore O_2 is empty. Lemma 1 says that the center O_2 and its neighbourhood are never nearer to an

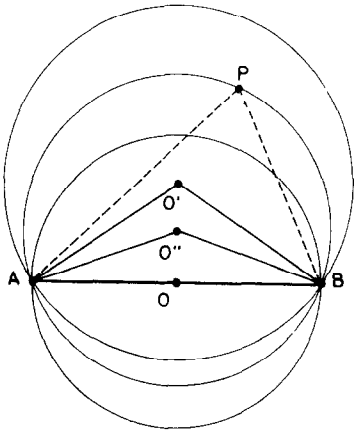

FIG. 7. See Lemma 3.

atom outside O_2 than to any of i, i_1, and i_2. Three perpendicular bisector planes $\{i, i_1\}$, $\{i, i_2\}$, and $\{i_1, i_2\}$ meet at O_2 and divide its neighbourhood into three Voronoi regions of i, i_1, and i_2. Therefore these three atoms are mutually contiguous. Q.E.D.

Proof of Theorem 3. Let O_3 be the circumsphere of the tetrahedron $\{i, i_1, i_2, i_3\}$. Two spheres O_2 and O_3 intersect with each other. The sphere O_2 is empty as shown in the proof of Theorem 2. If atom j were outside O_2 and inside O_3, the circumradius of the tetrahedron $\{i, i_1, i_2, j\}$ would be smaller than that of $\{i, i_1, i_2, i_3\}$ according to Lemma 3. This contradicts the condition. Therefore O_3 is empty. Lemma 1 says that the center O_3 and its neighbourhood are never nearer to an atom outside O_3 than to any of i, i_1, i_2, and i_3. Then the tetrahedron $\{i, i_1, i_2, i_3\}$ is a DT. Q.E.D.

Proof of Theorem 4. Let O_4 be the circumsphere of the tetrahedron $\{i, i_\alpha, i_\beta, i_\gamma\}$. Let O_5 be the circumsphere of the tetrahedron $\{i, i_\alpha, i_\beta, i_\delta\}$. The intersection circle of the two spheres O_4 and O_5 is the circumcircle of the triangle $\{i, i_\alpha, i_\beta\}$. The sphere O_4, which is the circumsphere of a DT, is empty. If atom j were outside O_4 and inside O_5, the circumcenter of the tetrahedron $\{i, i_\alpha, i_\beta, j\}$ would lie between O_4 and O_5 according to Lemma 2. In other words, it would have a smaller Z-coordinate value than O_5. This contradicts the condition. Then the sphere O_5 is empty. Lemma 1 says that the center O_5 and its neighbourhood are never nearer to an atom outside O_5 than to any of i, i_α, i_β, and i_δ. Therefore the tetrahedron $\{i, i_\alpha, i_\beta, i_\delta\}$ is a DT.

Q.E.D.

6. Further Details

Selection of S_i

In Section 3, we described how to find C_i, T_i, and then Π_i for a given set S_i. The efficiency of the algorithm depends on the selection of S_i. The selection of too large an S_i wastes computing time. Too small an S_i ($C_i \not\subset S_i$) leads to a wrong construction of Π_i. The optimal choice of S_i depends on the type of configuration of atoms.

Our interests are mainly concerned with the configuration of atoms in condensed phases, i.e., liquid, amorphous, and solid, and the coexistence of these. In such cases, the shape of Voronoi polyhedra is expected to be spherical. Then, S_i is selected to be a set of the nearest N_s atoms to $\mathbf{x}_i$. We take $N_s \cong 40$ since the number of faces of polyhedra is empiricaly in the range 10–20. Taking the density fluctuation into account, we search the nearest N_s atoms inside the sphere which contains about $2N_s$ atoms on average.

The check of whether this selection of S_i leads to the correct construction of Π_i is done in the following manner. Let d_i be the distance of the furthest vertex of Π_i from atom i. Then, if the distance of the N_sth atom from atom i is greater than $2d_i$, the construction of Π_i is consistent. Otherwise we must increase N_s for atom i until this condition is satisfied.

Problems Concerning Boundaries

Our algorithm was designed originally to analyze the atomic configurations of a system confined in a cube, which are generated by computer experiment with a periodic boundary condition. Then the whole space is covered by replicas of the original cube and the extended system has translational symmetry.

One is often interested in a system without such a feature, for example, a finite system in which all atoms are localized in some region of space. To apply our algorithm to this system we construct a cube which encloses the region. The effect of the periodic boundary condition appears only for Voronoi polyhedra in the region near the box surface. One can pick up such affected Voronoi polyhedra by examining, for the concerned atoms, whether or not the contiguous atoms are in the original box, or by inspecting the shape or size of their Voronoi polyhedra.

Degenerate Case

If five or more atoms happen to be on a spherical surface and if this sphere is empty, then this corresponds to a degenerate case mentioned in Section 2. In this case, the Voronoi tessellation is also unique, although Voronoi polyhedra of the five or more atoms meet at the center of this sphere. Some of these polyhedra are not normal in the following sense: four or more faces meet at a vertex. In the nondegenerate case, three faces meet at every vertex of any Voronoi polyhedron, which we call a normal polyhedron. The Delaunay tessellation for the degenerate case is different from that for a nondegenerate case: a certain polyhedron other than tetrahedron appears, which is inscribed in the above mentioned sphere. Any division of this polyhedron into tetrahedra leads to a Delaunay tessellation by tetrahedra alone, thus the "tetrahedral" Delaunay tessellation is not unique in a degenerate case.

Our algorithm gives a consistent set T_i of DT for Π_i in this case, because we search DT's sequentially so that any additional DT has a face in common with a previously found DT. Therefore, our algorithm gives a correct Voronoi tessellation.

Removal of Degeneracy

There is another treatment of the degenerate case. The degeneracy is removed if only a small amount of displacement is given to the atoms which are members of the degenerate set. Then there remains no ambiguity in the Delaunay tessellation, the Voronoi tessellation in the concerned region changes, and all the Voronoi polyhedra are normal.

Different displacements from one degenerate configuration lead to different

are rhombic dodecahedra in which degeneracy takes place at six vertices among fourteen. If the atoms are randomly displaced, the rhombic dodecahedra change into various kinds of polyhedra and the crystalline order is difficult to see. If the system of atoms is compressed along the (1 0 0) axis, the degeneracy is removed and all the Voronoi polyhedra are tetrakaidecahedra, as for a BCC lattice [7].

Our program has two options: treatment by random displacements and by compression along the (1 0 0) axis.

Dynamical Problems and Degeneracy

Though degeneracy happens very rarely in a given static configuration, it takes place not only in regular lattices but also in dynamical problems of atomic systems. From a dynamical point of view, the Voronoi tessellation changes only through an instantaneous degenerate configuration. Then the degeneracy is not a trivial exceptional case. A detailed study of degenerate cases yields a classification of configurations in terms of Voronoi tessellation (Ogawa [9]).

7. Efficiency of the Algorithm

In order to compare the efficiency of our algorithm with other algorithms, we prepared two programs; one is that of Finney [4] and the other is that of Brostow *et al.* [3]. The former is easy to program because of the simple structure of the algorithm. The latter is available to us from the authors by request. We evaluated the mean execution time for construction of a single polyhedron for the same configurations of $N = 500$. Figure 8 shows the results for several values of N_s. It is

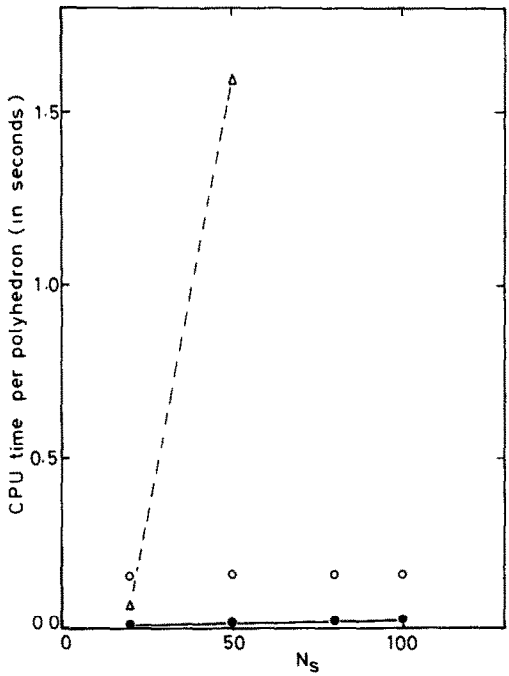

FIG. 8. Estimated computing time per Voronoi polyhedron against several values of N_s. The symbol (●) corresponds to ours, (○) to Brostow *et al.*, (△) to Finney. Values for Finney's algorithm are 0.075, 1.591, 7.007, and 14.163 for $N_s = 20$, 50, 80, and 100, respectively. Values for our algorithm and that of Brostow *et al.* are given in Tables I and II. The configuration used for these estimations is that of a metastable liquid with density $\rho = N/V = 1.10$ and $N = 500$. See [7] for details.

evident that our algorithm is fairly efficient when compared to the other two algorithms. In the figure, for the algorithm of Brostow *et al.* [3], the dependence of computing time on N_s is nearly as small as ours. It is also obvious that Finney's algorithm is generally much less efficient.

Let us analyse the dependence on N_s for each algorithm. Our algorithm starts with constructing an initial DT on the basis of Theorems 1–3. The number of operations to get the initial DT is proportional to N_s (steps 1–3 in Section 3). In step 4, we detect another atom as the fourth vertex of a new DT for a fixed bottom triangle and the condition is examined at most N_s times. The algorithm is to find DT's sequentially. Then the number of computations to obtain the complete set T_i and the Voronoi polyhedron Π_i of atom i is approximately vN_s, where v is the number of vertices of Π_i, i.e., the number of DT's in T_i. The computing time for each step is presented in Table I.

Finney's algorithm constructs DT's as we do. However, his program constructs tetrahedra for all the possible sets of three atoms among N_s atoms, together with the central atom. The number of sets is ${}_{N_s}C_3$. Only a tetrahedron whose circumsphere is empty is a DT. To distinguish a DT from the others, cN_s computations are required on the average, where c (< 1) is a positive numerical factor. Then the computation time is proportional to N_s^4.

The algorithm by Brostow *et al.* consists of the following three steps: (I) finding a set of direct neighbors (FACFIN), (II) constructing a polyhedron from the set (DIRPOL), and (III) constructing the Voronoi polyhedron (VORPOL). In (I), whether an atom can be a direct neighbour or not is judged by simply checking the

TABLE I

Composition of Computing Time per Voronoi Polyhedron for Our Algorithm

N_s	Selection of S_i and Step 1	Step 2 and Step 3	Step 4	Total	Step 5
20	0.00176 (18.5%)	0.00324 (34.1%)	0.00450 (47.4%)	0.00950	0.00182
50	0.00238 (16.5%)	0.00442 (30.6%)	0.00763 (52.9%)	0.01443	0.00182
80	0.00365 (18.2%)	0.00570 (28.4%)	0.01072 (53.4%)	0.02007	0.00183
100	0.00807 (28.9%)	0.00675 (24.2%)	0.01312 (46.9%)	0.02794	0.00189

Note. The unit of computing time is given in seconds. For the meaning of each step, see Section 3. The values in the last column "Step 5" are the same for all algorithms and "total" does not include the time of Step 5.

TABLE II

Composition of Computing Time per Voronoi Polyhedron for the Algorithm by Brostow *et al.*

N_s	Selection of S_t and Step (I)	Step (II)	Step (III)	Total
20	0.00388 (2.7%)	0.10606 (72.6%)	0.03610 (24.7%)	0.14604
50	0.00602 (4.1%)	0.10497 (71.5%)	0.03591 (24.4%)	0.14690
80	0.00755 (5.1%)	0.10465 (70.7%)	0.03591 (24.2%)	0.14801
100	0.01109 (7.3%)	0.10452 (69.0%)	0.03585 (23.7%)	0.15146

Note. For the meaning of each step, see text.

sign of a linear function. If the number of the direct neighbours is f_d, the number of conditions to be checked is approximately $(\frac{1}{2})f_d N_s$. In (II), $2f_d - 4$ vertices of the direct polyhedron are determined only after $f_d^4/6$ examinations. In (III), the procedure to find the contiguous atoms among the other $N_s - f_d$ atoms requires about $(f + f_d - 4) \cdot (N_s - f_d)$ examinations, where f is the number of faces of Π_t. Whenever a new candidate for a contiguous atom is found, the new vertices are calculated to prepare the examinations for the other succeeding atoms. Sometimes the candidates may turn out not to be contiguous afterwards. After all these procedures, the Voronoi polyhedron is determined. Though step (I) is simple and short, (II) and (III) are rather long. The computing time for each step is presented in Table II.

Our procedure is always based on the fact that some atoms are surely contiguous. We always detect only one atom at every step. Well-established theorems enable us to avoid the repeated computations proportional to N_s^n where $n > 2$. That is the reason why our algorithm is more efficient than others. All of the computations for the estimation of computing time were done on a HITAC M-200H of the Institute of Statistical Mathematics. Our program requires about 1300 FORTRAN statements, including I/O statements and comments. The amount of storage necessary for this is 300 kilobytes, for which systems of up to 4000 atoms are adaptive.

8. Possible Improvement and a Generalization

In the present algorithm, each Voronoi polyhedron is independently constructed. Therefore, strictly speaking, it is not an algorithm for computing the Voronoi tessellation itself but for repeated construction of a single Voronoi polyhedron. This repetition can be avoided by registering information about a Voronoi polyhedron at

the first construction and by utilizing it later. The total number of DT's is $(f/2-1)N < 7N$ if the average number of faces of a Voronoi polyhedron is f in an N-atom system and if the modest estimation $f \lesssim 16$ is used. If all atoms concerning a DT are registered, the total number of the required memory is $(2f-4)N < 28N$. The computing time will be reduced to less than one fourth, since the construction of an initial DT need be done only once and since its construction takes more computing time than that of another DT (see Table I). The algorithm now involves only computing the Voronoi tessellation.

This improvement is a natural extention of the algorithm. In the present algorithm, the guiding principle of closing a polyhedron is that each triangular face of the DT's that contain the central atom as their common vertex is used twice. In the improved algorithm, the Voronoi tessellation is complete when and only when all DT's are used four times.

From another point of view, the construction of a Voronoi polyhedron can be regarded as a tessellation of a closed surface into triangles. The tetrahedral DT tessellation of a space, which is in one-to-one correspondence with a Voronoi tessellation, can be regarded as a tessellation of a closed three-dimensional hypersurface of a four-dimensional region into tetrahedra when periodic boundary conditions are imposed. It means that the algorithm can be very naturally extended for any dimension and the number of required computations is always proportional to N_s, irrespective of the dimensionality.

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