

Voronoi diagram of 3D spheres: theory and applications

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ABSTRACT

Voronoi diagrams have several important applications in science and engineering. While the properties and algorithms for the ordinary Voronoi diagram of point set have been well-known, their counterparts for a set of spheres have not been sufficiently studied. In this paper, we present the definition, properties and algorithms for the Voronoi diagram of 3D spheres based on the Euclidean distance from the surface of spheres. Then, we show how such a Voronoi diagram can be used for solving various important geometric problems in biological systems.

Key words: Voronoi diagram, Euclidean, algorithm, molecular surface, interaction interface

1 INTRODUCTION

Since its introduction in the early 20th century, the Voronoi diagram has been one of the central topics in computational geometry as well as in other disciplines in science and engineering. The ordinary Voronoi diagram for a point set and its construction have been studied extensively in both 2 and higher dimensions [13]. However, the construction of the Voronoi diagram for spheres in Euclidean distance metric, often referred to as an *additively weighted Voronoi diagram* [13], has not been explored sufficiently even though the potential impact of this Voronoi diagram on diverse applications can be significant [1,5,11,15,17].

There are many important applications for such a Voronoi diagram. For example, the structural analysis of protein requires an efficient computational tool to analyze the spatial structure among its atoms [5,6,15]. In the design of new material, a similar analysis is fundamental as well [10,12]. Despite of its applicability to various problems, the previous studies are very limited [2,18,4,10]. Recently, Kim et al. reported on the details of an edge-tracing algorithm and its full implementation for constructing the whole Voronoi diagram with discussions on various applications including the analysis of protein structures [6–8].

In this paper, we present properties and two algorithms for Voronoi diagram of 3D spheres based on the Euclidean distance from the surface of spheres. Then, we show how such a Voronoi diagram can be used for solving various important geometric problems in biological systems.

2 DEFINITIONS RELATED TO THE EUCLIDEAN VORONOI DIAGRAMS FOR SPHERES

Let $S = \{s_1, s_2, \dots, s_n\}$ be a set of generators where s_i is a three dimensional spherical ball. Hence, $s_i = (c_i, r_i)$ where $c_i = (x_i, y_i, z_i)$ and r_i denote the center and radius of a ball,

respectively. We assume that no ball is completely contained inside another ball while other types of intersections between balls are allowed. Associated with each ball s_i , there is a corresponding region VR_i , called a *Voronoi region* for s_i , where $VR_i = \{p | dist(p, c_i) - r_i \leq dist(p, c_j) - r_j, i \neq j\}$. Then, $VD(S) = \{VR_1, VR_2, \dots, VR_n\}$ is called the *Euclidean Voronoi diagram* for S . In this paper, the ordinary L_2 -distance from the surface of balls is used to define Euclidean Voronoi diagrams.

Illustrated in Fig. 1(a) and (b) are fifteen balls with three different radii and the Voronoi region corresponding to the largest ball in the center. Fig. 1(c) shows the Voronoi diagram of a subset of protein with 67 atoms, which form an alpha-helix, downloaded from PDB [14].

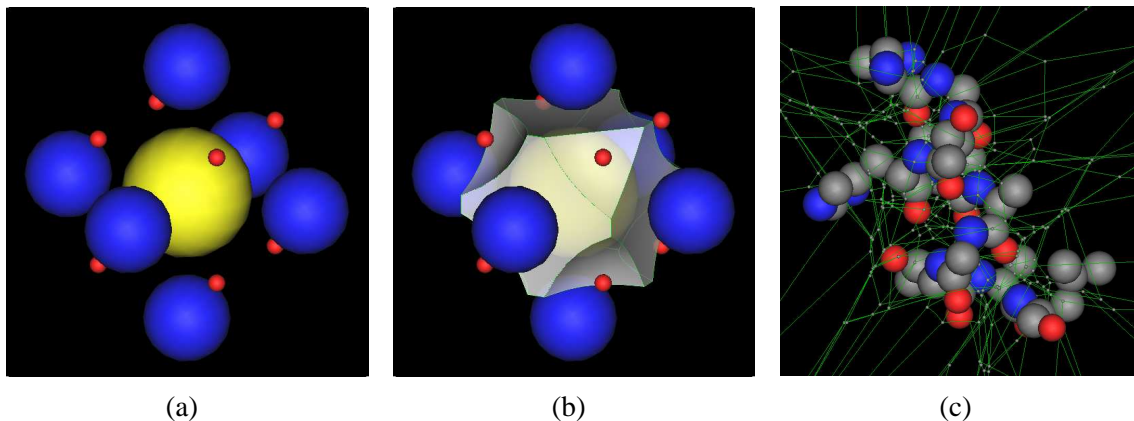


Figure 1. Voronoi diagrams

3 ALGORITHMS FOR $VD(S)$

A Voronoi vertex is the center of an empty sphere simultaneously tangent to four balls. A Voronoi edge is defined as the locus of points equi-distant from three nearby balls, and it can be easily shown that an edge is always a conic curve and can be conveniently represented, if necessary, in a rational quadratic Bézier form [8]. Two topologically neighboring balls define a Voronoi face as a locus of points equi-distant from two nearby balls, and the face is a segment of a hyperboloid of two sheets and its equation can be easily obtained [5,8].

3.1 Edge-Tracing Algorithm

The idea of the edge-tracing algorithm is simple as it constructs Voronoi edges in the order of a depth-first search. The algorithm first locates a true Voronoi vertex v_0 by computing an empty tangent sphere defined by four appropriate nearby balls. Given v_0 , four edges e_0, e_1, e_2 , and e_3 emanating from v_0 can be easily identified and pushed into a stack called an *Edge-stack*. Hence, these edges have v_0 as their starting vertices. After popping an edge from the stack, the algorithm computes the end vertex of the popped edge. Note that the end vertex can be found by computing an empty sphere tangent to four balls: three balls which define the popped edge and one of the $(n - 3)$ candidate balls. If an empty tangent sphere is found, the center of the sphere may become the end vertex of the popped edge. Once the end vertex of edge is found, it is also possible to define three new edges emanating from this new vertex. Hence, these new edges starting from the new vertex just computed are created and pushed into the Edge-stack. By following this process until the Edge-stack is empty, the computation of the Voronoi diagram of a connected graph is completed.

Given an initial Voronoi vertex to start with, the edge-tracing algorithm runs in $O(mn)$ time in the worst-case, where m is the number of edges and n is the number of balls. The algorithm iterates $O(m)$ times since it traces all edges once for each edge. For each edge, it is necessary to do $O(n)$ scans through all candidate balls once to compute a valid tangent sphere.

3.2 Region-Expansion Algorithm

The region-expansion algorithm extends its precursor in 2D and adapts the idea of discrete event simulation. Let $VD(P)$ be an ordinary Voronoi diagram of the centers of balls. The algorithm constructs $VD(S)$ by expanding Voronoi regions for one ball after another via a series of edge-flips, starting from $VD(P)$. After choosing a point generator c_i , which is the center of a spherical ball s_i , and the corresponding Voronoi region VR_i , the algorithm continuously enlarges the point generator c_i to the ball s_i . Then, the corresponding region VR_i expands according to the enlargement of the corresponding generator. Repeating the process for all generators constructs a correct Voronoi diagram if the topology is consistently and correctly maintained.

The computation necessary to expand a Voronoi region, starting from a center point to a complete ball, takes $O(n^2 \log n)$ time in the worst-case since there can be $O(n^2)$ number of edges and sorting is necessary according to the event time of each edge. Therefore, the whole Voronoi diagram can be constructed by the region-expansion algorithm in $O(n^3 \log n)$ time in the worst-case. We believe, however, that there should be a tighter bound for the worst-case time complexity and the expected time complexity can be much lower.

4 APPLICATIONS OF $VD(S)$ IN BIOLOGICAL PROBLEMS

4.1 Computation of Molecular Surfaces

A protein is usually modelled as a set of hard spheres in order to represent atoms in a *space-filling model* where their radii are the van der Waals radii [3,9]. Given such a model, there are usually two kinds of surfaces involved: a *solvent accessible surface(SAS)* and a *molecular surface(MS)*. A SAS, first defined by Lee and Richards [9], is the set of centers of a spherical probe rolling around the protein. A probe is used for the computational convenience of a small molecule which interacts with the protein.

A MS, also known as a *Connolly surface*, consists of the most inward points on the probe toward the interior of a protein when the probe is in contact with two or more atoms in the protein [3,16]. It is well-known that atoms located at the boundary of a protein determine the function of the protein. Hence, knowledge of a molecular surface is important in the study of protein functions since the surface has a direct relation with other atoms.

The molecular surface consists of two groups: a *solvent contact surface(SCS)* and a *reentrant surface(RS)*. A SCS consists of points on the van der Waals atoms which are touchable by a probe. A RS is defined as points on the inward part of the surface of a probe, where the probe is in contact with atoms [16]. An RS, known as a blending surface in CAGD community, consists of two types of blending surface patches: *rolling blending* and *link blending*. These blending surface patches can be computed by rolling a spherical probe in every possible direction while keeping tangential contact with the atoms.

It turns out that a $VD(S)$ conveniently stores all information necessary for the computation of the molecular surface of a protein. Shown in Fig. 2(a) is a subset of protein data downloaded from PDB [14] which forms an α -helix. In the model, there are 41 C's, 14 N's, and 12 O's.

Fig. 2(b), (c) and (d) show the molecular surfaces defined by different probes with radii of 1.4Å, 4Å, and 8Å, respectively. Note that all molecular surfaces are computed from the identical Euclidean Voronoi diagram of the model in Fig. 2(a).

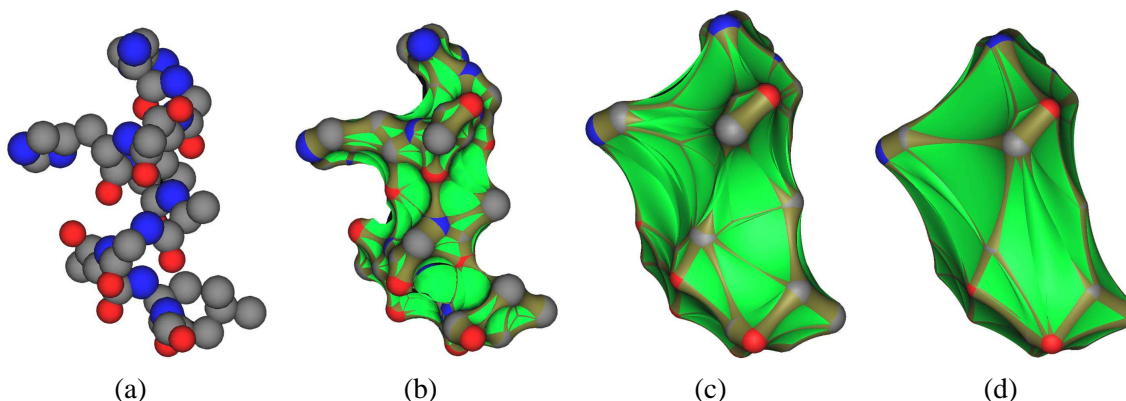


Figure 2. Molecular surfaces

4.2 Analyzing Interaction Interfaces

A protein is a macromolecule consisting of the permutation of 20 different kinds of amino acids. Amino acids are linearly connected to one another via peptide bonds to form chains. When a protein consists of two chains, it is called a *dimer* as shown in Fig. 3(a). Shown in Fig. 3(b) and (c) are examples of a *trimer* (three chains) and a *tetramer* (four chains), respectively. Since interaction among chains is critical for protein functions, understanding the interaction is getting more important and the geometric properties of the interactions are getting more attention.

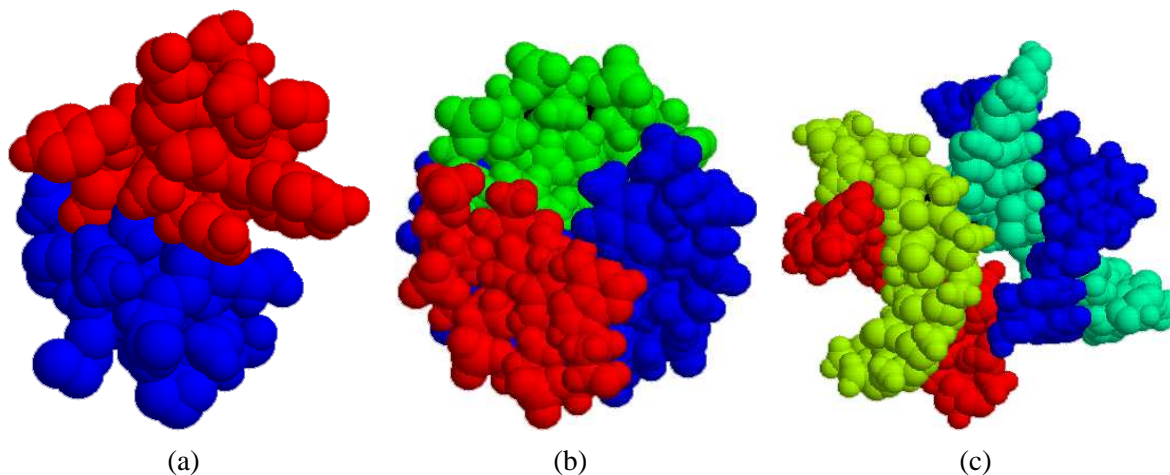


Figure 3. Protein examples: (a) a dimer, (b) a trimer, and (c) a tetramer.

The *interaction interface IIF* is defined in this paper as follows. Let $A = \{a_1, a_2, \dots, a_m\}$, $B = \{b_1, b_2, \dots, b_n\}$ be two chains in a protein, where a_i and b_j are atoms with appropriate centers and radii. The interaction interface between two chains A and B is defined as $IIF_\infty(A, B) = \{p \mid dist(p, A) = dist(p, B)\}$, where $dist(p, A)$ denotes the minimum Euclidean distance from p to the surfaces of all van der Waals atoms in the set A . Then, $IIF_\infty(A, B)$ is a subset of Voronoi faces in $VD(A \cup B)$. Hence, $IIF_\infty(A, B)$ can be easily located by simply

checking each Voronoi face with its generating atom types. Note that $IIF_{\infty}(A, B)$ expands to infinity.

The infinite Voronoi faces in $IIF_{\infty}(A, B)$ are biologically less significant since proteins, as well as $IIF_{\infty}(A, B)$, are usually hydrated. Hence, we define a *trimmed interaction interface* $IIF(A, B)$ against a probe of a water molecule. Fig. 4(a) and (b) illustrate the van der Waals atoms of a dimer 1bh8 downloaded from PDB and the corresponding $IIF(A, B)$, respectively.

To analyze the topology and geometry of an interaction interface, we define a *base surface* $BS(A, B)$ which is defined as a smooth surface fitted through the trimming curve of $IIF(A, B)$ with a certain minimality condition. Fig. 4(c) shows the base surface $BS(A, B)$ of $IIF(A, B)$ in Fig. 4(b). Once an interface and its corresponding base surface are obtained, various analyses can be done on the interaction behavior between chains in the protein.

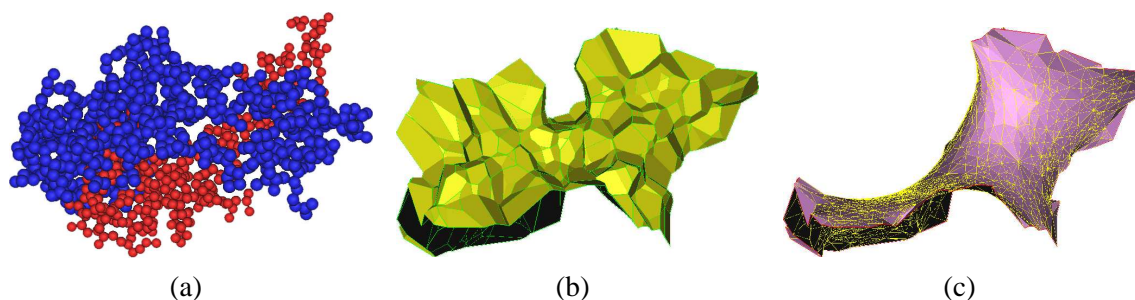


Figure 4. A dimer (PDB ID: 1bh8): (a) van der Waals model, (b) IIF , and (c) BS .

5 CONCLUSIONS

In this paper, we have presented properties and two algorithms for Voronoi diagram of 3D spheres based on the Euclidean distance from the surface of spheres. We have also shown how such a Voronoi diagram can be used for solving various important geometric problems in biological systems by illustrating two examples: the computation of surfaces defined on a protein, and the extraction and characterization of interaction interfaces between multiple proteins.

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