International Journal of CAD/CAM Vol. 7, No. 1, pp. 91~101 (2007)

INTERNATIONAL JOURNAL OF CAD/CAM
www.ijcc.org

β-Shape and β-Complex for the Structure Analysis of Molecules

Jeongyeon Seo[1], Donguk Kim[2], Youngsong Cho[3], Joonghyun Ryu[3] and Deok-Soo Kim[1]*

[1]*Department of Industrial Engineering, Hanyang University, Korea*

[2]*Department of Industrial & Systems Engineering, Kangnung National University, Korea*

[3]*Voronoi Diagram Research Center, Hanyang University, Korea*

Abstract – To understand the structure of molecules, various computational methodologies have been extensively investigated such as the Voronoi diagram of the centers of atoms in molecule and the power diagram for the weighted points where the weights are related to the radii of the atoms. For a more improved efficiency, constructs like an α-shape or a weighted α-shape have been developed and used frequently in a systematic analysis of the morphology of molecules. However, it has been recently shown that α-shapes and weighted α-shapes lack the fidelity to Euclidean distance for molecules with polysized spherical atoms. We present the theory as well as algorithms of β-shape and β-complex in $\mathbb{R}^3$ which reflects the size difference among atoms in their full Euclidean metric. We show that these new concepts are more natural for most applications and therefore will have a significant impact on applications based on particles, in particular in molecular biology. The theory will be equivalently useful for other application areas such as computer graphics, geometric modeling, chemistry, physics, and material science.

Keywords **: Voronoi diagram of spheres, quasi-triangulation, α-shape, β-shape, structural biology**

1. Introduction

The topology among particles frequently plays a core role in many applications. In particular, particles are important in computer graphics, GIS, biometrics, etc. An immediate example is to interpolate a surface from a point cloud where the proximity information among neighboring points is necessary. One of the emerging application areas of particle systems is structural molecular biology since the morphology of a molecule is one of the most important factors to determine the functions of the molecule.

The topological characteristics among particles have been long time questions in mathematics, science and engineering. Due to the lack of a proper representation, in old days, the studies on the topological characteristics among particles were primarily done by either investigating all pairwise comparisons or employing a simple grid or a bucket. In 1967, Bernal and Finney used the Voronoi diagram of points, where the points are the centers of spheres, to analyze the packing characteristics of spherical particles such as the distributions of particle density, the number of Voronoi faces for Voronoi cells, and the number of Voronoi edges for Voronoi faces. [4]. Since then, many studies have followed in the studies of geometric and topological characteristics of molecular systems and the Voronoi diagram of points has been extensively used. In 1974, Richards used the Voronoi diagram of atom centers to estimate the volume of the space that each atom or a group of atoms in protein occupies, etc. [33]. Since then, until today, there have been numerous studies in physics, chemistry, biology, and various other fields which use the Voronoi diagram of atom centers [1,8,30,40,42].

While the size differences among atoms are significantly meaningful, the Voronoi diagram of atom centers does not reflect the size differences. In 1982, Gellatly and Finney proposed to use a radical plane as the bisector between two atoms so that the space occupied by a set of polysized atoms is properly tessellated [14]. This transformation is later named the power diagram of atoms by Aurenhammer [2] since the distance metric of the tessellation using radical planes is indeed a power distance. Since then, the power diagram has been very popular in the analysis of systems of polysized particles in science and engineering [16,28,37,41].

On the other hand, the concept of α-shape in $\mathbb{R}^2$ was proposed as a generalization of the convex hull of a point set and was used to define the shape of the point set [12,13]. The idea was based on a transformation from the Delaunay triangulation which is a topological dual of the Voronoi diagram of points [13]. Even though it is powerful for points, the α-shape does not reflect the size differences among spherical particles at all as it is based on the Voronoi diagram of points. Hence, the concept was later extended to a weighted α-shape which is based on the regular triangulation, the dual of power diagram [9]. However, it turns out that the power diagram still has limitations for the queries based on Euclidean distance metric.

Recently the theory of β-shape and β-complex, which are respectively generalizations of the ordinary α-shape and α-

*Corresponding author:
Tel: +82-2-2220-0472
Fax: +82-2-2292-0472
E-mail: dskim@hanyang.ac.kr

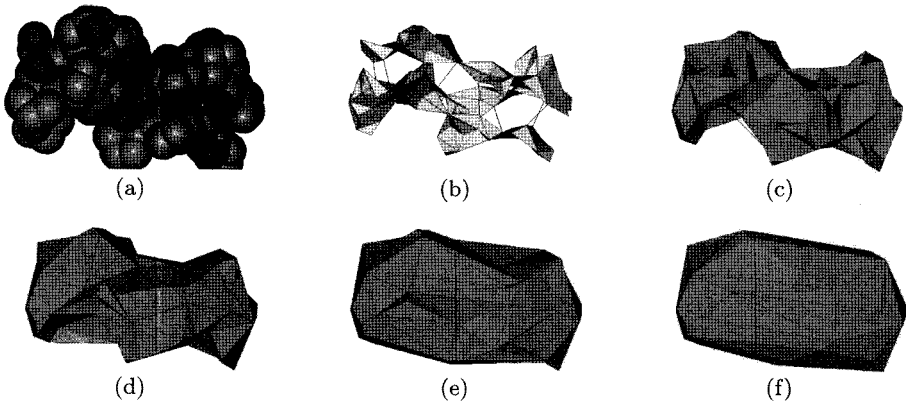


Fig. 1. The β-shapes for a protein via different β-values: (a) a protein (PDB ID: 1v4f) consisting of 133 atoms (different colors denote different atoms 84 C's, 28 O's and 21 N's), (b) the β-shapes with $\beta = 0$, (c) $\beta = 0.7$Å, (d) $\beta = 1.4$Å, (e) $\beta = 5$Å, and (f) $\beta = 50$Å.

complex, was proposed and used as a powerful tool for understanding proximity among particles [24,38]. The β-complex is based on the quasi-triangulation which is the dual structure of the Voronoi diagram of spheres (also known as an additively weighted Voronoi diagram). We believe that the β-shape will be more applicable to many problems based on Euclidean distance metric. Fig. 1 shows different β-shapes with respect to different β-values from the protein shown in Fig. 1(a) which is downloaded from the Protein Data Bank (PDB) [32].

This paper is organized as follows. In Section 2, we briefly review the Voronoi diagram of spheres and its dual structure called a quasi triangulation, which are the basis of the β-complex. Section 3 presents the theory of β-family consisting of β-hull, β-shape, and β-complex. Section 4 explains the algorithms to compute a β-complex and its data structure. In Section 5, we provide several applications of β-complex to biological problems such as the molecular surface construction, pocket extraction and various mass property computations. Finally, we conclude the paper.

2. Related works

The theory of β-complex is a generalization of the ordinary α-complex. The α-complex is computed from the Delaunay triangulation which is the dual structure of the Voronoi diagram of points. In a similar method, β-complex is computed from the quasi-triangulation which is the dual structure of the Voronoi diagram of spheres. In this section, we describe the Voronoi diagram of spheres, frequently known as an additively weighted Voronoi diagram, and its dual called a quasi-triangulation.

2.1 Voronoi diagram of spheres and quasi-triangulation

A Voronoi diagram VD(S) for the sphere set S is defined as VD(S) = {VC(s_1),VC(s_2), ..., VC(s_n)} where the connectivity among the entities are appropriately represented. Associated with each sphere $s_i \in S$, there is a corresponding *Voronoi cell (or region)* $VC(s_i)$ for s_i, where $VC_i = \{p \mid dist(p, c_i) - r_i \leq dist(p, c_j) - r_j, i \neq j\}$, where $dist(p, q)$ denotes Euclidean distance between points p and q. In $\mathbb{R}^3$, VD(S) consists of $V^V = \{v_1^V, v_2^V, ...\}$, $E^V = \{e_1^V, e_2^V, ...\}$, $F^V = \{f_1^V, f_2^V, ...\}$, and $C^V = \{c_1^V, c_2^V, ... c_n^V\}$ which denote the sets of Voronoi vertices, Voronoi edges, Voronoi faces, and Voronoi cells (or regions) in the Voronoi diagram VD(S), respectively. From the definition of a Voronoi diagram, a Voronoi vertex v^V is the center of an empty sphere tangent to four nearby atoms, while a Voronoi edge e^V is defined as a locus of points equi-distant from the surfaces of three surrounding atoms. In addition, a Voronoi face f^V is the surface defined by two neighboring atoms. Note that the face is always a hyperbolic surface and any point on the face is equi-distant from the surfaces of both atoms. For more details, readers are recommended to refer to [20,21,22].

In the cases of the Voronoi diagram of points or the power diagram, their respective dual complexes are well-defined as the Delaunay and the regular triangulations. However, the dual of the Voronoi diagram had not been discussed until it was recently reported by Kim et al. [23]. A *quasi-triangulation* QT(S) is defined as QT(S) = {τ_1, τ_2, ..., Δ_1, Δ_2, ...} where τ and Δ denote a tetrahedron and a triangle, respectively, which are the dual cells in the quasi-triangulation QT(S), where the topology is appropriately represented. Note that a dual cell in QT(S) may degenerate to a triangle [23].

Let $V^Q = \{v_1^Q, v_2^Q, ... v_n^Q\}$, $E^Q = \{e_1^Q, e_2^Q, ...\}$, $F^Q = \{f_1^Q, f_2^Q, ...\}$, and $C^Q = \{c_1^Q, c_2^Q, ...\}$ denote the sets of vertex simplexes, edge simplexes, face simplexes, and cell simplexes in QT(S), respectively. Then, a quasi-triangulation QT(A) for an atom set A can be conveniently represented as QT(A) = (V^Q, E^Q, F^Q, C^Q). A Voronoi diagram VD(A) is mapped to a quasi-triangulation QT(A) as follows.

- A Voronoi cell $c^V \in C^V$ is mapped to a vertex $v^Q \in V^Q$. The vertex v^Q corresponds to the center of a generator atom a_i corresponding to a Voronoi cell c^V.
- A Voronoi face $f^V \in F^V$ is mapped to an edge $e^Q \in E^Q$. The edge e^Q is a line segment bounded by two v^Q's.
- A Voronoi edge $e^V \in E^V$ is mapped to a face $f^Q \in F^Q$. The face f^Q is a triangle bounded by three e^Q's.
- A Voronoi vertex $v^V \in V^V$ is mapped to a cell $c^Q \in C^Q$. The cell c^Q is a tetrahedron bounded by four f^Q's.

The dual structure QT(A) is called a quasi-triangulation since it is not always a valid triangulation of R^3 space. Recall that the topological duals of the Voronoi diagram of points and the power diagram are called the Delaunay triangulation and the regular triangulation, and both triangulations are simplicial complexes which tessellate the convex hull of input points by a set of tetrahedra. If they do intersect, two tetrahedra in these triangulations intersect each other at a vertex, an edge, or a triangular face. In QT(A), however, this property is not guaranteed.

2.2 InterWorld Data Structure (IWDS) for quasi-triangulation

Since a quasi-triangulation QT(A) is not a simplicial complex in general, it is usually stored as a primal structure, i.e. the Voronoi diagram of the atom set A [5]. Recently, a method has been proposed to directly store QT(A) in a set of simple arrays which is called an *InterWorld data structure*, abbreviated as *IWDS* [23]. It was shown in [23] that the IWDS compactly stores the topology of QT(A) with a guaranteed query efficiency.

In [23], it was shown that there are three kinds of anomalies which cause the violation of the definition for simplexes to form a complex: a multiplicity anomaly, a singularity anomaly, and a degeneracy anomaly. By coping with the anomalies in the quasi-triangulation, which are surprisingly less frequent, the compact IWDS is devised to store the topology of a quasi-triangulation as a straightforward extension of the array-based data structure for a simplicial complex [23]. IWDS maintains one more relatively small array in addition to the array for simplicial complexes: a *gate* array. The multiplicity anomaly and the degeneracy anomaly are handled by appropriately adjusting the values in the elements of arrays and the singular anomaly is handled by the gate array signifying the singularity. For the details, please refer to [23].

IWDS stores the complete information about the topology of QT(S) in the most compact way. It can be used for both representing the topology of QT(S), or equivalently VD(S), in a code and storing QT(S) or VD(S) in a file. When we use it in codes, however, we slightly extend IWDS to facilitate a more convenient manipulation of the simplexes. The extension called an *extended* IWDS, denoted by *eIWDS*, is done by introducing two more arrays to IWDS: edge and face arrays. In eIWDS, the gate array is not necessary any more since the gate information can now be stored in the corresponding edge.

In eIWDS, the entities of quasi-triangulation in a neighborhood are interconnected in a straight forward manner. A vertex has a pointer to one of the incident edges, and an edge has a pointer to one of the incident faces and two pointers to its two vertices. A triangular face has two pointers to the two tetrahedra which share the face and three pointers to the three edges bounding the face. A tetrahedron has four pointers to the four bounding triangular faces. With eIWDS, any pair of two adjacent entities in QT(S) can be traversed with at most three hops via pointers.

3. β-family

Recently the theory of β-complex was proposed and used as a powerful tool for understanding proximity among particles. Although the α-complex has been widely used in variety of applications due to its theoretical beauty and simplicity, it does not property account for size difference among given spheres from the viewpoint of Euclidean distance. In comparison, the β-complex fully considers the Euclidean fidelity to particles sizes. First, in this section, we explain the β-family which is composed of β-hull, β-shape, and β-complex. Then, we provide a great asset of β-complex in the Euclidean metric.

3.1 β-hull and β-shape

Conceptually, a β-hull is the generalization of an α-hull and can be similarly described. The point set, from which an α-hull is defined, is now replaced by a set of three dimensional spherical balls. As for the case of α-hulls, think of $\mathbb{R}^3$ filled with Styrofoam and some spherical rocks scattered around inside the Styrofoam. The radii of the spherical rocks vary. Then, carving out the Styrofoam with an omnipresent and empty spherical eraser with the radius of β will result in a β-hull. Since the eraser is omnipresent, there can be interior voids as well. The molecular surface, used in biology quite a long time, is indeed equivalent to the β-hull of the molecule [6,7]. Figs. 2(a) and 2(d) show an identical atom set in the plane and two β-hulls or molecular surfaces corresponding to two erasers with different sizes. Let us call these erasers the β-probe.

Suppose that we have a β-hull of an atom set A. Then, we straighten the surface of the β-hull by substituting straight edges for the circular ones and triangles for the spherical caps where the vertices are the centers of the atoms contributing to the β-hull. Then, the straightened object is the *β-shape* of A. Figs. 2(b) and 2(e) illustrate two β-shapes corresponding to the two β-hulls in Figs. 2(a) and 2(d), respectively.

3.2 β-complex

Suppose that $\tilde{A} \subseteq A$ where $|\tilde{A}| = k+1$ where k is the dimension of the space for the centers of atoms $\alpha \in \tilde{A}$ are defined. Note that $k+1$ center points define k-dimensional simplex due to the general position assumption. Let $b_{\tilde{A}}$ be the smallest empty open β-probe whose boundary $\partial b_{\tilde{A}}$ touches all atoms of $\tilde{A}$ from outside. Let $\rho_{\tilde{A}}$ be the radius of $b_{\tilde{A}}$. Hence, $2 \le |\tilde{A}| \le 4$ in the three-dimensional space since $1 \le k \le 3$. The case of $k=0$ is defined specially since $b_{\tilde{A}}$ in this case trivially reduces to a point and the corresponding atom always maps to a vertex simplex.

Definition 1 *For* $1 \le k \le 3$ *and* $0 \le \beta \le \infty$, *let* $\Sigma^C_{k,\beta}$ *be the set of k-simplexes* $\sigma_{\tilde{A}}$ *in the β-complex for which a β-probe* $b_{\tilde{A}}$ *is empty and* $\rho_{\tilde{A}} \le \beta$. *Especially,* $\Sigma^C_{0,\beta} = C$ *for any value of β, where* $C = \{c_1, c_2, \ldots, c_n\}$ *is the set of atom centers. Then, a β-complex* C_β *is defined as* $C_\beta = \{\sigma_{\tilde{A}'} \mid \sigma_{\tilde{A}} \in \Sigma^C_{k,\beta}, \tilde{A}' \subset \tilde{A}, 0 \le k \le 3\}$.

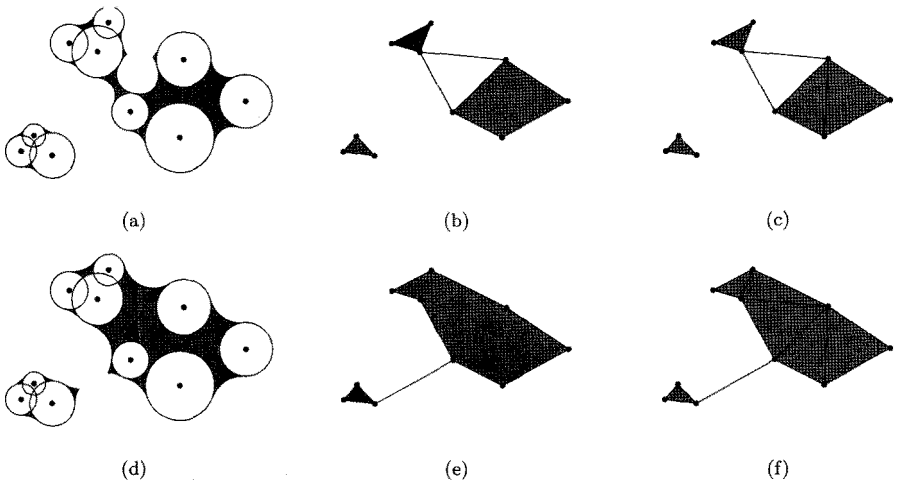


Fig. 2. β-hulls, β-shapes and β-complexes for the atoms in $\mathbb{R}^2$: (a) ten two-dimensional atoms and the β-hull corresponding to a small β-probe with β_1, (d) the β-hull of the same atom set corresponding to a large β-probe with β_2 where $\beta_1 < \beta_2$, (b) and (e) the β-shapes corresponding to β_1 and β_2, and (c) and (f) the β-complexes by β_1 and β_2.

Therefore, a β-complex C_β is defined as the set of either k-simplexes $\sigma_{\tilde{A}}$ in $\Sigma^C_{k,\beta}$ or those k-simplexes which bound $(k+1)$-simplexes in C_β. In addition, each simplex in a β-complex C_β may take one of the following three states depending on the value of β.

Definition 2 *A simplex σ in a β-complex C_β takes one of the following three bounding states.*

- singular: *σ belongs to the boundary of β-shape S_β and does not bound any higher-dimensional simplex in the corresponding β-complex C_β.*
- regular: *σ belongs to the boundary of β-shape S_β* and *bounds at least one higher-dimensional simplex in the corresponding β-complex C_β.*
- interior: *σ does not belong to the boundary of β-shape S_β, and σ is the intersection between neighboring simplexes of higher dimensions in the corresponding β-complex C_β.*

The β-complex of an atom set A is a subset of simplexes in the quasi-triangulation of A where the volume union of the simplexes in the β-complex is identical to the corresponding β-shape. Shown in Figs. 2(c) and 2(f) are the β-complexes of the β-shapes in Figs. 2(b) and 2(d), respectively. As shown in the figure, each β-shape is tessellated into a set of simplexes. A simplex σ in a β-complex takes one of the above three bounding states [38]. Note that a simplex has one of these states if it belongs to a β-complex. Note that β-shape is defined as a subset of the underlying space of all the simplexes in β-complex where the underlying space of simplexes means the union of the spaces occupied by the simplexes. Therefore, we can say that the β-shape can be obtained from the corresponding β-complex and the β-complex fully contains the information of β-shape.

Also, a simplex can be one of the following two situations depending on the condition of the smallest possible tangent sphere Z which is simultaneously tangent to the atoms corresponding to the vertices of the simplex from outside.

Definition 3 *A simplex σ is classified according to the following intersection cases.*

- *σ is unattached if there is no intersection between Z and any atom in A.*
- *σ is attached if there is an intersection between Z and some atom in A.*

The valid intervals of β values for each simplex are shown in Table 1. Let CH(A) denote the convex hull of whole atoms in the atom set A, and CH(C) denote the convex hull of the centers of all atoms in A. In addition, let $\widetilde{CH}(A)$ denote the polytope defined by the centers of atoms which contribute to CH(A). When there is a cylindrical boundary between a pair of atoms in CH(A), a corresponding edge is defined in $\widetilde{CH}(A)$ between the centers of the two atoms. When there is a triangular boundary for a triplet of atoms in CH(A), a corresponding triangle is defined in $\widetilde{CH}(A)$ among the centers of the three atoms. Note that $\widetilde{CH}(A)$ is not identical to CH(C) in general.

All simplexes $\sigma_{\tilde{P}} \in \mathrm{QT}(A)$ have their respective intervals according to the singular, regular, or interior states in the complex C_β. $\sigma_{\tilde{P}}$ is a simplex of the β-complex C_β iff β is contained in this interval. A regular simplex belongs to the boundary of the interior of β-shapes. In a β-complex, a regular simplex bounds some higher-dimensional simplexes while a singular simplex does not. The interior simplexes triangulate the interior of β-shapes.

The meaning of the rules in Table 1 can be explained as follows. First, a tetrahedron simplex σ, Case 1 in the table, is defined and remains as interior after a minimum empty sphere tangent to a set of four atoms in $\tilde{A}$ is found. Note that σ can be only interior, if it is an element of a β-complex.

Case 2 denotes an edge or a face simplex which is not on the boundary of the convex hull and unattached and needs a little bit of explanation. The other cases can be similarly explained. Let $\tilde{A} = \{a_i, a_j\}$, $1 \le i, j \le n$, $i \ne j$, $\tilde{A}' = \tilde{A} \cup \{a_k\}$, and $\tilde{A}'' = \tilde{A} \cup \{a_l\}$, $i \ne j \ne k \ne l$. Suppose that $\sigma_{\tilde{A}'}$ and $\sigma_{\tilde{A}''}$ are two triangles among others incident to an edge simplex $\sigma_{\tilde{A}}$.

Table 1. The set of rules that transforms simplexes in the quasi-triangulation to β-complex

		Case	Bounding State		
			Singular	Regular	Interior
Tetrahedron		1			$(\rho_{\tilde{A}}, \infty]$
Edge or triangle	$\notin \partial\,\widetilde{CH}(A)$, Unattached	2	$(\underline{\rho}_{\tilde{A}}, \underline{\mu}_{\tilde{A}}]$	$(\underline{\mu}_{\tilde{A}}, \overline{\mu}_{\tilde{A}}]$	$(\overline{\mu}_{\tilde{A}}, \infty]$
	$\notin \partial\,\widetilde{CH}(A)$, Attached	3		$(\underline{\mu}_{\tilde{A}}, \overline{\mu}_{\tilde{A}}]$	$(\overline{\mu}_{\tilde{A}}, \infty]$
	$\in \partial\,\widetilde{CH}(A)$, Unattached	4	$(\underline{\rho}_{\tilde{A}}, \underline{\mu}_{\tilde{A}}]$	$(\underline{\mu}_{\tilde{A}}, \infty]$	
	$\in \partial\,\widetilde{CH}(A)$, Attached	5		$(\underline{\mu}_{\tilde{A}}, \infty]$	
	Isolated triangle	6	$(\underline{\rho}_{\tilde{A}}, \overline{\rho}_{\tilde{A}}]$		
Vertex	$\notin \partial\,\widetilde{CH}(A)$	7	$[-\infty, \underline{\mu}_{\tilde{A}}]$	$(\underline{\mu}_{\tilde{A}}, \overline{\mu}_{\tilde{A}}]$	$(\overline{\mu}_{\tilde{A}}, \infty]$
	$\notin \partial\,\widetilde{CH}(A)$	8	$[-\infty, \underline{\mu}_{\tilde{A}}]$	$(\underline{\mu}_{\tilde{A}}, \infty]$	

In addition, suppose that $0 < \rho_{\tilde{A}'} < \rho_{\tilde{A}''} < \infty$, and the radius ρ corresponding to any other triangle incident to $\sigma_{\tilde{A}}$ satisfies $\rho_{\tilde{A}'} < \rho < \rho_{\tilde{A}''}$. Then, $\underline{\mu}_{\tilde{A}} = \rho_{\tilde{A}}$ and $\overline{\mu}_{\tilde{A}} = \rho_{\tilde{A}''}$.

Suppose $\rho_{\tilde{A}} < \beta \le \underline{\mu}_{\tilde{A}}$. Then, an empty β-probe can keep its tangency with the two atoms a_i and a_j. This means that the β-probe does not intersect with any other atom in the atom set A. Hence, the edge $\sigma_{\tilde{A}}$ is defined in the β-complex while no triangle incident to the edge is defined. The edge $\sigma_{\tilde{A}}$ A is singular since it exists as a singleton. Note that, when the value of β is in this range, neither $\sigma_{\tilde{A}'}$ nor $\sigma_{\tilde{A}''}$ is a triangle in the β-complex yet.

Suppose that $\underline{\mu}_{\tilde{A}} < \beta \le \overline{\mu}_{\tilde{A}}$. Then, $\sigma_{\tilde{A}'}$ becomes a triangle and is an element in β-complex while the other triangle $\sigma_{\tilde{A}''}$ is not defined yet in β-complex. Since the edge $\sigma_{\tilde{A}'}$ bounds a triangle $\sigma_{\tilde{A}'}$ in this case, the edge is called regular. If $\overline{\mu}_{\tilde{A}} < \beta \le \infty$, the edge simplex $\sigma_{\tilde{A}}$ A is in the interior of β-complex because the two incident triangles $\sigma_{\tilde{A}'}$ and $\sigma_{\tilde{A}''}$ are now the elements of β-complex and the edge is shared by the two triangles. Note that the edge $\sigma_{\tilde{A}}$ A does not even exist if $\beta \le \rho_{\tilde{A}}$.

Suppose that $\sigma_{\tilde{A}}$ A is now a face simplex which can be similarly explained to the previous edge case. In other words, $\sigma_{\tilde{A}}$ A is a 2-σ. Then, an explanation similar to the above can be made.

In this case, $\sigma_{\tilde{A}'}$ and $\sigma_{\tilde{A}''}$ are appropriately defined tetrahedra sharing $\sigma_{\tilde{A}}$.

Given the rules in the above table, the following two lemmas can be derived to compute the β-complex and β-shape for a given value of β.

Lemma 1 *The β-complex for a particular value of β consists of simplexes in QT(A) iff the β is contained in one of the β-intervals for three bounding states shown in Table 1.*

Lemma 2 *The boundary of the β-shape consists of the simplexes in the β-complex whose bounding states* are either singular or regular for a particular value of β.

Proof: As mentioned previously, the β-shape is a subset of the underlying space of β-complex. According to the rule for transforming simplexes in the quasi-triangulation to a β-complex in Table 1, interior simplexes be enclosed by all their incident higher dimensional simplexes except for a tetrahedron. In addition, the highest simplex in 3D, i.e. tetrahedron, always has interior state. Hence, the interior simplexes cannot contribute to the boundary of β-shape. Therefore, the boundary of the β-shape consists of either singular or regular simplexes in the β-complex.

In addition, the boundary of the β-shape cannot be directly computed by locating the boundary of the Euclidean space occupied by the elements in a β-complex. However, Lemma 2 provides an algorithm to compute the boundary of a β-shape correctly and efficiently from a corresponding β-complex.

3.3 Euclidean fidelity of β-shape and β-complex

Now, the Euclidean fidelity to particle size of β-complex is explained. The α-shape and α-complex have a limitation for being used in biological applications since they cannot account for the size difference among particles. In order to incorporate the size differences among particles, an extended concept called the weighted α-shape was proposed [9]. The weighted α-shape is based on the regular triangulation of the particles, which is the dual of the corresponding power diagram. However, the weighted α-shape based on the power diagram also has limitations for queries based on Euclidean distance metric although they reflect the size variations of atoms at a certain level. Fig. 3(a) shows a set of 2D atoms with different sizes and the power diagram defined on the atom set. Fig. 3(b) shows its counterpart for the Voronoi diagram of atoms where the distance is defined as the minimum Euclidean distance from a point to the boundary of atoms. The dotted circle in Fig. 3(a) is a tangent circle which is computed from the three atoms a_1, a_2, and a_3 corresponding to a vertex v_1 in the power diagram. Note that the tangent circle intersects with the atom a_4. On the other hand, the dotted tangent circle in Fig. 3(b) corresponds to the Voronoi vertex v_2 in the

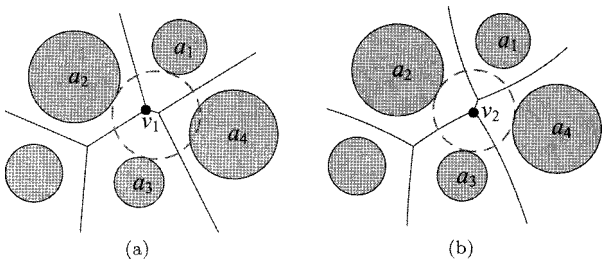


Fig. 3. Discrepancy between power diagram and Voronoi diagram.

Voronoi diagram of atoms and is guaranteed to be intersection-free with any other atoms. Therefore, the largest empty circle in the atomic structure can easily be found by a simple scan through the vertices of the Voronoi diagram. However, the same computation is not well-defined in the power diagram and a search, not necessarily local, is necessary.

Goede et al. criticizes that the power cell is not always chemically reasonable particularly for bonded atoms due to the fact that a power cell may not include the corresponding input point [15]. Shown in Fig. 4 is an example of the cell inclusion. Let r_H and r be the radii of an hydrogen atom H and an arbitrary atom, respectively, and d be the distance between the centers of these two atoms. Then, it is easy to show that the power cell of H does not contain the center of H, if the following inequality holds. This observation indeed indicates the inappropriateness of the weighted α-shape in the analysis of molecular structure and suggests a desperate need for a new construct based on the Voronoi diagram of atoms for the correct analysis of a molecular structure [15,31].

$$r > \sqrt{r_H^2 + d^2} \tag{1}$$

Suppose that the radius of H is 1.2Å and there are three types of bonding between H and, for example, a carbon atom C which correspond to three different values of d [18]: (a) 1.09Å, (b) 1.06Å, and (c) 1.08Å. Since the radius of C is known as 1.7Å, the power cell of any hydrogen atom does not contain the center of the hydrogen regardless of the bonding type in nature. Other atoms also frequently lead to similar situations.

4. Algorithms for a β-shape and a β-complex

Suppose that a quasi-triangulation is stored in the data structure of eIWDS. Given a value of β, the corresponding β-complex and β-shape can be extracted from the quasi-triangulation by Lemma 1 and Lemma 2, respectively. The extractions are done by searches among the simplexes whose β-intervals contain β. In our earlier algorithm, a β-shape was computed directly from the Voronoi diagram of atoms [24] and this approach turned out to be memory intensive and inconvenient. The previous algorithm was devised in that way due to the lack of understanding of the dual structure and the data structure to represent the dual.

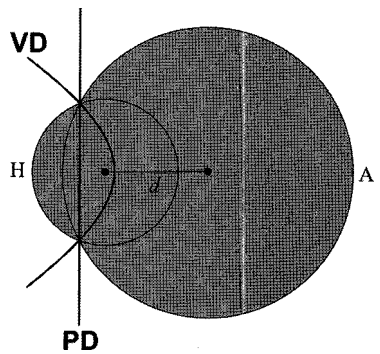


Fig. 4. Cell Inclusion. The power cell of the hydrogen atom does not contain the center of the hydrogen while the Voronoi region does contain the center.

Suppose that we want to compute a β-complex corresponding to a particular value of β. Then, we have to locate all simplexes which contain β within their β-intervals. The result of the search for β-complex may consist of 0-, 1-, 2-, and/or 3-σ's and the states of simplexes may be either singular, regular or interior. Suppose that we treat each simplex as a distinct and a unique entity in the sorted set and use the start value of the β-intervals of a simplex as the key for the sorting. Then, a standard sorting algorithm takes $O(\Sigma_{d=0}^{3} m_d \log m_d)$ for m_d d-σ simplexes in the quasi-triangulation. Recall that a simplex has at most three β-intervals. Suppose we want to compute the boundary of a β-shape. Then, the first obvious approach is to compute a β-complex and remove the interior simplexes. A better approach, however, would be to do a search of the singular and regular simplexes directly on the sorted arrays of 0-, 1-, and 2-σ's. We do not need to consider 3-σ's for the search since 3-σ only contributes to the interior.

When a value of β is given, we can search an initial simplex (which is either singular or regular) σ_0 from, for example, the array for vertices V^Q via a binary search which takes $O(\log |V^Q|)$ time. Suppose that there are k_V singular or regular vertex simplexes defining the boundary of a β-shape. Then, the other $k_V - 1$ vertex simplexes are in the consecutive neighborhood of σ_0 in the array. Therefore, a linear scan from σ_0 locates all the other vertex simplexes defining the boundary of the β-shape. Hence, the search takes $O(\log |V^Q| + k - 1)$ time. We do a similar process for the edge and face simplexes as well. Hence, the whole search can be done in $O(\log |V^Q| + \log |E^Q| + \log |F^Q| + k_V + k_E + k_F - 3)$ time. If we maintain all related simplexes in a single array of size m and the boundary of β-shape consists of k simplexes, the time complexity is given as $O(m \log m + k)$.

5. Applications in Molecular Biology

The topology among particles frequently plays a core role in many applications. One of the emerging application areas of particle systems is the analysis of molecular structure since the morphology of a molecule has been recognized as one of the most important factors which determines the functions of the molecule. Therefore, the β-shape and the β-complex can play a key role in solving many problems analyzing molecular structure of atomic complexes. Once the β-shape and β-complex are computed for a given value of β for a given atom set A, many analyses related to the structure of A can be done very precisely, efficiently and conveniently. To show the capabilities of β-shape and β-complex, the following examples are provided.

5.1 Molecular Surface Construction

An important geometric measure of a molecule is its molecular surface. The computation of *molecular surface* is also important in the study of molecular structure [6,7] and

the topology among atoms is the most fundamental part of the efficient computation of molecular surface.

Lee and Richards were the first who defined the concept of a solvent accessible surface of a protein. Using this concept, they were able to compute the free space that the center of a probe can move around without touching the protein [25]. Richards also initially defined the molecular surface of protein [34]. Since then, several computational studies of the surfaces on a protein have been conducted.

Connolly later computed the molecular surface of a protein to calculate the protein volume, electrostatic potential, and interface surfaces between molecules. The approach was to compute some sample points on the molecular surface to approximate the true surface [7]. Connolly also presented an analytic representation of a molecular surface [6] where he pointed out that a molecular surface consists of three types of patches: a convex spherical patch, a saddle-shaped toroidal patch, and a concave spherical patch.

Once a β-shape is computed, the molecular surface for a given probe of size β can be easily computed. Ryu et al. presents the algorithm which is summarized as a lemma below [35,36].

Lemma 3 Let σ be *a* simplex in a β-shape. Then, a molecular surface is define by the following.

- *If σ is a singular vertex, the complete atom corresponding to σ is on the molecular surface.*
- *If σ is a singular edge, a complete rolling blending patch is defined between two atoms corresponding to the vertices of σ.*
- *If σ is a regular edge, a partial rolling blending patch is defined between two atoms corresponding to the vertices of σ.*
- *If σ is a singular face, two pieces of triangular link patch is defined between three atoms which correspond to the vertices of σ.*
- *If σ is interior, the atoms corresponding to the vertices of σ do not contribute to the molecular surface.*

Corollary 4 *Given a β-shape consisting of k simplexes, the molecular surface corresponding to the β-shape can be computed in O(k) time in the worst case.*

For the details, [35,36] should be referred to. Since a molecular surface can be computed in a linear time with respect to the number of atoms using a β-shape, the molecular surfaces corresponding to a probe with varying size can also be efficiently computed. The experiment shows that the molecular surfaces can be visualized in a realtime-like speed.

However, if a weighted α-shape is used, a problem similar to finding the largest empty circle, as shown in Fig. 3, occurs [3]. To alleviate the difficulty for the weighted α-shape, the atoms have to be enlarged by some amount, the power diagram should be computed again, the regular triangulation should be found, and the corresponding weighted β-shape should be computed. Therefore, if we want to compute different molecular surfaces corresponding to different probes, it is necessary to compute different power diagrams again and again. Bajaj reported a study on the range of probe radius which can compute the corresponding molecular surfaces with one power diagram [3]. To the contrary, the Voronoi diagram of atoms needs to be computed only once regardless of the probe radius since the Voronoi diagram is unique for a set of atoms and can be used for any probe.

Experiments have been done via a full implementation of the presented algorithm using several protein models available from Protein Data Bank (PDB) [32]. Fig. 5(a) shows a protein 1apm and Fig. 5(b) shows its molecular surface defined by a water molecule which is approximated by a probe of 1.4Å radius. Different colors denote different types of atoms and therefore different sizes. Figs. 5(c) and 5(d) illustrate molecular surfaces of the same protein corresponding to probes of different sizes.

It is important that the three molecular surfaces in Figs. 5(b), 5(c), and 5(d) are all computed from the three corresponding β-shapes which are quickly computed from a single QT(A), therefore a single VD(A), of the protein. We also would like to note that the number of blending patches in a molecular surface increases as the probe size decreases. For example, the number of the blending patches in Fig. 5(b) is much larger than that of Fig. 5(d). However, the average size of patches in Fig. 5(d) is much larger than that of Fig. 5(b).

5.2 Docking Site Extraction

Given two molecules, analyzing interactions between them is important for understanding their biological interactions. The interaction between a protein and a small molecule is indeed

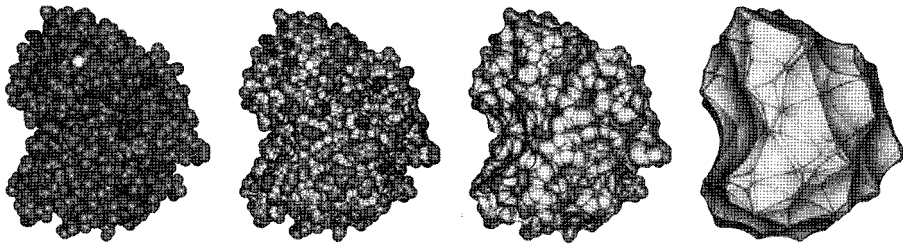


Fig. 5. Protein model and its molecular surfaces. (a) a protein model (The catalytic Subunit of Camp-dependent Protein Kinase Complexed with a Peptide Inhibitor and Detergent, PDB id: 1apm) (b) a molecular surface corresponding to a probe with 1.4Å, (c) a molecular surface corresponding to a probe with 2.8Å, and (d) a molecular surface corresponding to a probe with 12.6Å.

one of the most important issues in designing new drugs. The study of molecular interactions, such as the docking of a protein with a ligand or protein folding, can be approached from a physicochemical or a geometrical point of view, or both [29].

A docking between a protein, called a *receptor*, and a small molecule, called a *ligand*, usually occurs around depressed regions, called *docking sites or pockets*, on the surface of a receptor. Since designing a new drug requires finding a small chemical which can dock or bind at pockets on a protein, the recognition of pockets on proteins is one of the most fundamental processes in drug design. Considering that chemical databases usually contain millions of chemical data entries, manually identifying pockets on the surface of a protein is time-consuming and error-prone. Therefore, the automatic recognition of pockets and the evaluation of the binding of a chemical to a pocket are rather important in the study of protein-ligand docking for the development of new drugs [39].

While the efforts on the physicochemical approach on this issue have been given since the early days of science, efforts to understand the geometry perspective of biological systems have started only very recently [11,17,25,27]. In the representation of the surface of an atomic structure, it is no doubt to say that β-shape is one of the most powerful tools. Kim et al. [19] reported an algorithm to extract depressed regions on the boundary of a protein by using two β-shapes defined by small and large β values. The β-shape defined by a small β value is called an inner β-shape and one defined by a large β is called an outer β-shape. We observed that the difference between the two β-shapes can define pockets of a given protein. In addition, for each edge of the outer β-shape, there is zero or one depressed region on the boundary of the protein. When an edge of the outer β-shape coincides with one of the inner β-shape, obviously no pocket is defined.

Fig. 6 shows the procedure of the pocket recognition. Shown in Fig. 6(a) is the input protein (PDB ID: 1 fkg) displayed by its molecular surface. Figs. 6(b) and 6(c) are the inner and outer β-shapes, respectively. The two β-shapes are overlapped in Fig. 6(d). The outer β-shape, in this example, is when β is ∞ and therefore it corresponds to the convex hull of the atoms. Note that a user can determine appropriate β values for inner and outer β-shapes as a parameter of the algorithm. Fig. 6(e) shows subdivided regions on the boundary of the inner β-shape and 6(f) shows the extracted pocket.

5.3 Mass Property Computation

Once a β-shape and the corresponding β-complex are given for a molecule, various analyses about the mass properties on the molecule can be done rather easily and efficiently. Volume and surface area of the union of spheres can be efficiently computed by β-complex. Edelsbrunner showed that the volume of the union of atoms can be efficiently and correctly computed by referring to the intersections among atoms via the weighted α-complex when α is zero [10]. Liang et al. applied this property to the molecular volume and area computation [26]. Since the weighted α-shape is identical with the β-shape when $\alpha = \beta = 0$, the same method can be used with the β-shape. If the corresponding

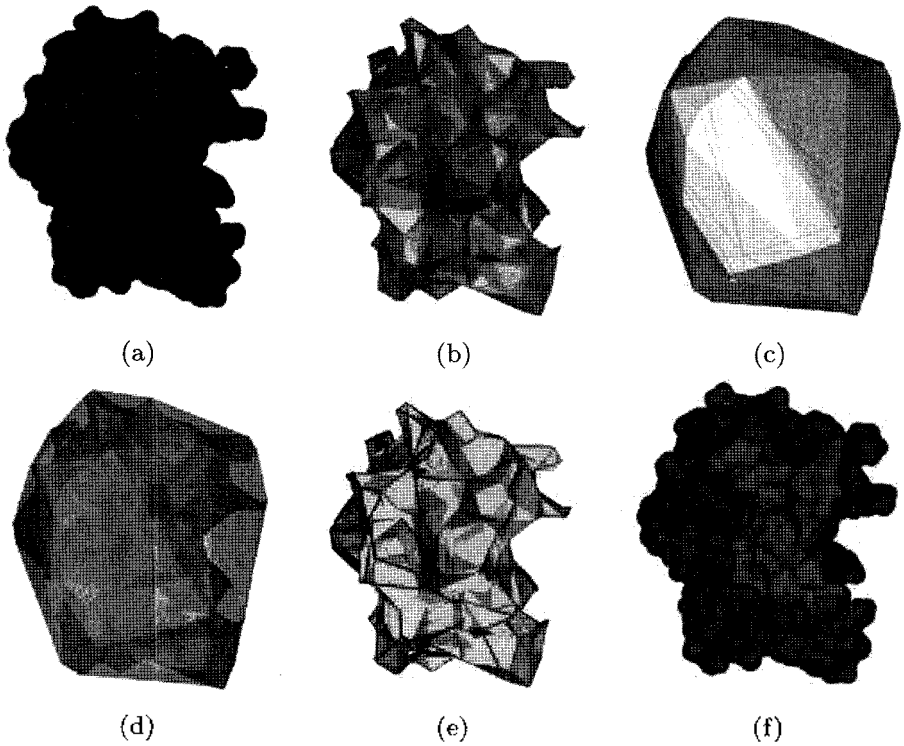


Fig. 6. Pocket extraction procedure: (a) a protein (PDB ID: 1 fkg), (b) inner β-shape, (c) outer β-shape, (d) overlap of inner and outer β-shapes, (e) subdivided regions on the boundary of the innerβ-shape, and (f) extracted pocket.

Table 2. The volume (unit: Å^3) and the surface area (unit: Å^2) of van der Waals models of the ten test proteins and their respective computation time (unit: sec). (Environment: Intel 3.2 GHz CPU, 2GB RAM and Windows XP OS)

	Model				
	1cgd	1hpv	1f6o	1ke5	2por
No. of atoms	604	1551	2154	2269	2306
Volume (A)	6,330.00	16,957.45	22,879.69	24,673.51	24,923.43
Surf. area (B)	7,393.25	20,388.04	26,930.60	29,400.41	29,980.04
Comp. time (A)	0.0060	0.0110	0.0177	0.0200	0.0171
Comp. time (B)	0.0057	0.0109	0.0175	0.0198	0.0169

β-complex is given, it can be used to compute the volume of the union of the van der Waals atoms of the molecule. The topology information among the simplexes in the β-shape and β-complex are used to set up the set operations for the computation. Table 2 shows the computation results of the surface area and the volume of van der Waals models for the protein and their respective computation times. Note that the number of atoms are also given in the table. The computation time was measured after the β-shapes and β-complexes are computed for the models.

6. Conclusions

In this paper, we discussed the β-shape and β-complex which generalize the well-known α-shape and α-complex (also their weighted counterparts as well) for a set of spheres with arbitrary sizes. Also, we showed that a number of important bio-problems such as the molecular surface construction, pocket extraction, and surface area and volume computation of a molecule can be efficiently solved via the concept of β-complex. After computing the Voronoi diagram of spheres, we transform the Voronoi diagram to a quasi-triangulation which is the topological dual of the Voronoi diagram. Then, an analysis for β-intervals is done with the quasi-triangulation to produce a simple rule to search in the intervals to compute the ?-complex as well as the β-shape.

The quasi-triangulation can be computed from the Voronoi diagram of spheres in $O(m)$ time in the worst case. Then, the presented theory and algorithms enable us to compute both β-complex and β-shape from the sorted array of simplexes in $O(\log m + k)$ time in the worst case, where the quasi-triangulation has m simplexes and the β-complex or β-shape has k simplexes, respectively.

Even though we mostly referred to applications for analyzing the structure of molecules such as proteins, the theory of β-shape and β-complex will be equally useful for other areas such as physics, chemistry, computer graphics, and geometric modeling where one of the fundamental issues is the proximity among particles.

Acknowledgements

J. Seo were supported by Korea Research Foundation Grant (KRF-2007-314-D00311). Y. Cho, J. Ryu and D.-S. Kim were supported by KOSEF through National Research Lab. (No. R0A-2007-000-20048-0).

References

[1] B. Angelov, J. F. Sadoc, R. Jullien, A. Soyer, J. P. Mornon, and J. Chomilier (2002), Nonatomic solvent-driven Voronoi tessellation of proteins: An open tool to analyze protein folds. Proteins: *Structure, Function, and Genetics*, **49**(4), 446-456.

[2] Aurenhammer, F (1987), Power diagrams: Properties, algorithms and applications. *SIAM Journal on Computing*, **16**, 78-96.

[3] Bajaj, C. L., Pascucci, V., Shamir, A., Holt, R. J. and Netravali, A. N (2003), Dynamic maintenance and visualization of molecular surfaces. *Discrete Applied Mathematics*, **127**(1), 23-51.

[4] Bernal, J. D. and Finney, J. L (1967), Random close-packed hard-sphere model ii. Geometry of random packing of hard spheres. *Discussions of the Faraday Society*, **43**, 62-69.

[5] Cho, Y., Kim, D. and Kim, D. S (2005), Topology representation for the Voronoi diagram of 3D spheres. *International Journal of CAD/CAM*, **5**(1), 59-68, (Also available at http://www.ijcc.org).

[6] Connolly, M. L (1983), Analytical molecular surface calculation. *Journal of Applied Crystallography*, **16**, 548-558.

[7] Connolly, M. L (1983), Solvent-accessible surfaces of proteins and nucleic acids. *Science*, **221**, 709-713.

[8] Dupuis, F., Sadoc, J. F. and Mornon, J. P (2004), Protein secondary structure assignment through Voronoi tessellation. *Proteins: Structure, Function, and Bioinformatics*, **55**, 519-528.

[9] Edelsbrunner, H (1992), Weighted alpha shapes. Technical Report UIUCDCS-R-92-1760, Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL.

[10] Edelsbrunner, H (1995), The union of balls and its dual shape. *Discrete & Computational Geometry*, **13**, 415-440.

[11] Edelsbrunner, H., Facello, M. and Liang, J (1998), On the definition and the construction of pockets in macromolecules. *Discrete Applied Mathematics*, **88**, 83-102.

[12] Edelsbrunner, H., Kirkpatrick, D. G. and Seidel, R (1983), On the shape of a set of points in the plane. *IEEE Transactions on Information Theory*, **IT-29**(4), 551-559.

[13] Edelsbrunner, H. and Mücke, E. P (January 1994), Three-dimensional alpha shapes. *ACM Transactions on Graphics*, **13**(1), 43-72.

[14] Gellatly, B. J. and Finney, J. L (1982), Calculation of protein volumes: An alternative to the Voronoi procedure. *Journal of Molecular Biology*, **161**(2), 305-322.

[15] Goede, A., Preissner, R. and Frömmel. C (1997), Voronoi cell: New method for allocation of space among atoms: Elimination of avoidable errors in calculation of atomic volume. *Journal of Computational Chemistry*, **18**(9), 1113-1123.

[16] Gong, S., Park, C., Choi, H., Ko, J., Jang, I., Lee, J. Bolser, D. M and D. O (August 2005), A protein domain interaction interface database: Interpare. *BMC Bioinformatics*, **6** (207).

[17] Heifets, A. and Eisenstein, M (2003), Effect of local shape modifications of molecular surfaces on rigid-body protein-protein docking. *Protein Engineering*, **16**(3), 179-185.

[18] Hopfinger, A. J (1973), *Conformational Properties of Macromolecules*. Academic Press.

[19] Kim, D.-S., Cho, C.-H., Kim, D. and Cho. Y (May 2006), Recognition of docking sites on a protein using β-shape based on Voronoi diagram of atoms. *Computer-Aided Design*, **38**(5), 431-443.

[20] Kim, D.-S., Cho, Y. and Kim. D (2005), Euclidean Voronoi diagram of 3D balls and its computation via tracing edges. *Computer-Aided Design*, **37**(13), 1412-1424.

[21] Kim, D.-S., Cho, Y., Kim, D. and Cho, C.-H (2004), Protein sructure analysis using Euclidean Voronoi diagram of atoms. In *Proceedings of the International Workshop on Biometric Technologies (BT2004)*, pages 125-129.

[22] Kim, D.-S., Cho, Y., Kim, D., Kim, S., Bhak, J. and Lee, S.-H (2004), Euclidean Voronoi diagram of 3D spheres and applications to protein structure analysis. In *Proceedings of the 1st International Symposium on Voronoi Diagrams in Science and Engineering (VD2004)*, pages 137-144.

[23] Kim, D.-S., Kim, D., Cho, Y. and Sugihara, K (2006), Quasi-triangulation and interworld data structure in three dimensions. *Computer-Aided Design*, **38**(7), 808-819.

[24] Kim, D.-S., Seo, J., Kim, D., Ryu, J. and Cho. C.-H (2006), Three-dimensional beta shapes. *Computer Aided Design*, **38**(11), 1179-1191.

[25] Lee, B. and Richards, F. M (1971), The interpretation of protein structures: Estimation of staticaccessibility. *Journal of Molecular Biology*, **55**, 379-400.

[26] Liang, J., Edelsbrunner, H., Fu, P., Sudhakar, P. V. and Subramaniam, S (1998), Analytical shape computation of macromolecules: I. molecular area and volume through alpha shape. *PROTEINS: Structure, Function, and Genetics*, **33**, 1-17.

[27] Liang, J., Edelsbrunner, H., Fu, P., Sudhakar, P. V. and Subramaniam, S (1998), Analytical shape computation of macromolecules: II. inaccessible cavities in proteins. *PROTEINS: Structure, Function, and Genetics*, **33**, 18-29.

[28] McConkey, B. J., Sobolev, V. and Edelman, M (1365), Quantification of protein surfaces, volumes and atom-atom contacts using a constrained Voronoi procedure. *Bioinformatics*, **18**(10):1365-1373.

[29] Parsons, D. and Canny, J (1994), Geometric problems in molecular biology and robotics. In *Proceedings of the 2nd International Conference on Intelligent Systems for Molecular Biology*, pages 322-330, California, USA, Stanford University.

[30] Pontius, J., Richelle, J. and Wodak, S. J (1996), Deviations from standard atomic volumes as a quality measure for protein crystal structures. *Journal of Molecular Biology*, **264**(1), 121-136.

[31] Poupon, A (2004), Voronoi and Voronoi-related tessellations in studies of protein structure and interaction. *Current Opinion in Structural Biology*, **14**, 233-241.

[32] RCSB Protein Data Bank Homepage. http://www.rcsb.org/pdb/.

[33] Richards, F. M (1974), The interpretation of protein structures: Total volume, group volume distributions and packing density. *Journal of Molecular Biology*, **82**, 1-14.

[34] Richards, F. M (1977), Areas, volumes, packing, and protein structure. *Annual Review of Biophysics and Bioengineering*, **6**, 151-176.

[35] Ryu, J., Park, R., Cho, Y., Seo, J. and Kim, D.-S (2007), *β-shape based computation of blending surfaces on a molecule. In Proceeding of the 4th International Symposium on Voronoi Diagrams in Science and Engineering (ISVD2007)*, pages 189-198.

[36] Ryu, J., Park, R. and Kim, D.-S (2007), Molecular surfaces on proteins via beta shapes. *Computer Aided Design*, **39**(12), 1042-1057, 2007.

[37] Sadoc, J. F., Jullien, R. and Rivier, N (2003), The laguerre polyhedral decomposition: Application to protein folds. *European Physical Journal B*, **33**, 355-363, 2003.

[38] Seo, J., Cho, Y., Kim, D. and Kim, D.-S (20070), An efficient algorithm for three-dimensional β-complex and β-shape via a quasi-triangulation. In *Proceedings of the ACM Symposium on Solid and Physical Modeling*, pages 323-328.

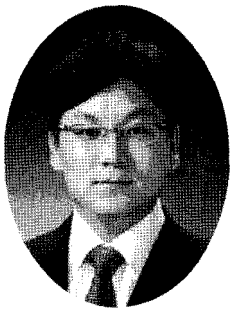
[39] Shoichet, B. K. and Kunts, I. D (1991), Protein docking and complementarity. *Journal of Molecular Biology*, **221**, 327-346.

[40] Tsai, J., Taylor, R., Chothia, C. and Gerstein, M (1999), The packing density in proteins: Standard radii and volumes. *J. Mol. Biol.*, **290**, 253-266.

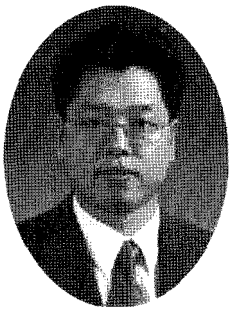
[41] Wernisch, L.., Hunting, M. and Wodak, S. J (1999), Identification of structural domains in proteins by a graph heuristic. *PROTEINS: Structure, Function, and Genetics*, **35**, 338-352.

[42] Zimmer, R., Wöohler, M. and Thiele, R (1998), New scoring schemes for protein fold recognition based on Voronoi contacts. *Bioinformatics*, **14**(3), 295-308.

Jeongyeon Seo

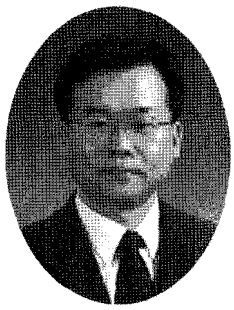


Donguk Kim



Youngsong Cho

Joonghyun Ryu



Deok-Soo Kim

Jeongyeon Seo is a Ph.D. student in Department of Industrial Engineering, Hanyang University, Korea. She received his B.S. and M.S. degrees from Hanyang University in 2004 and 2006, respectively. Her research interests include computational geometry, geometric modeling and their applications in the molecular biology.

Donguk Kim is an assistant professor in Department of Industrial and Systems Engineering, Kangnung National University, Gangneung, Korea. Before he joined the university, he worked at Voronoi Diagram Research Center at Hanyang University, Seoul, Korea. He received his B.S., M.S. and Ph.D. degrees from Hanyang University in 1999, 2001 and 2004, respectively. His research interests include geometric modeling, Voronoi diagrams and their applications in the molecular biology.

Youngsong Cho is a senior researcher in Voronoi Diagram Research Center at Hanyang University, Seoul, Korea. He received his B.S., M.S. and Ph.D. degrees from Hanyang University in 1995, 1997 and 2003, respectively. His research interests include computational geometry, geometric modeling and their applications in the molecular biology.

Joonghyun Ryu is a senior researcher in Voronoi Diagram Research Center at Hanyang University, Seoul, Korea. He received his B.S., M.S. and Ph.D. degrees from Hanyang University in 1997, 1999 and 2002, respectively. His research interests include computational geometry, geometric modeling and their applications in the molecular biology.

Deok-Soo Kim is a professor in Department of Industrial Engineering, Hanyang University, Korea. Before he joined the university in 1995, he worked at Applicon, USA, and Samsung Advanced Institute of Technology, Korea. He received a B.S. from Hanyang University, Korea, an M.S. from the New Jersey Institute of Technology, USA, and a Ph.D. from the University of Michigan, USA, in 1982, 1985 and 1990, respectively. His current research interests mainly lie in the theory and applications of Voronoi diagram while he has been interested in various geometric problems.He is current the director of Voronoi Diagram Research Center supported by the Ministry of Science and Technology, Korea.