

# Molecular surfaces of proteins based on $\beta$ -shapes and Voronoi diagrams of atoms

Joonghyun Ryu<sup>1</sup>, Rhohun Park<sup>2</sup>, Choel-Hyung Cho<sup>1</sup> and Deok-Soo Kim<sup>2</sup>

1) *Voronoi Diagram Research Center, Hanyang University, Seoul 133-791, KOREA*

2) *Department of Industrial Engineering, Hanyang University, Seoul 133-791, KOREA*

Corresponding Author : Deok-Soo Kim, dskim@hanyang.ac.kr

## ABSTRACT

Given the atomic complex of protein, it is important to understand the interactions among proteins. One of the approaches to the problem is to analyze the geometric structure of a protein because it is known that its geometric structure directly determines the protein functions. The molecular surface of the protein is one of the important geometric structure for the analysis of the protein. This paper presents an algorithm for precisely and efficiently computing the molecular surface of a protein using a proposed geometric construct called  $\beta$ -shape based on the Voronoi diagram of atoms in the protein. Given the Voronoi diagram of atoms based on the Euclidean distance from the atom surfaces, the proposed algorithm first computes a  $\beta$ -shape with an appropriate probe. Then, the molecular surface is computed by employing the blending operation on the atomic complex of the protein.

## SURFACE MODEL ON A PROTEIN

Protein consists of a set of amino acids and an amino acid contains different types of atoms. Therefore, a protein can be modeled by a set of 3D spheres, which corresponds to its constituting atoms. Given the atomic complex of a protein, one of the important geometric structures of a protein is the molecular surface of protein since a molecular surface distinguishes the interior and exterior of the protein and plays an important role in protein folding, docking, interactions between proteins, and so on [1–3].

Due to its importance, there have been several researches on geometric structures of a protein [4,5]. In this paper, we show that the molecular surface of the protein can be efficiently and conveniently computed via  $\beta$ -shape of atoms transformed from the Voronoi diagram of atoms in a protein. Note that the computation of Euclidean Voronoi diagram for 3D spheres could have been computed recently [6].

Protein is usually solvated in the water. Suppose we represent each water molecule contacted with the protein as an 3D sphere enclosing the water molecule. Then, we can define the molecular surface of a protein by rolling the enclosing sphere, which is called by *probe*, over the protein. There are two types of surfaces constituting the molecular surface. *Solvent contact surface* is the atom surface which the solvent molecule contact with. The most inward part of probe boundary is the *reentrant surface*, which is the *blending surface* of the protein by the given probe. In this paper, we recognize the topology of molecular surface and the types of its constituting surfaces by using the  $\beta$ -shape transformed from Voronoi diagram of atoms. Then,

the molecular surface is computed by employing the blending operation on the atomic complex of the protein.

### $\beta$ -SHAPE AND MOLECULAR SURFACE

Suppose that we are given with an atomic structure  $A$  and a probe  $p$ . Then, we connect the *centers* of the atoms with edges and triangles whenever a particular probe  $p$  in the space touches two or three nearby atoms simultaneously, respectively. Then, the  $\beta$ -shape corresponding to the probe  $p$  for a set  $A$  is obtained. If we apply this operation for all pairs or triplet of atoms, we can obtain both  $E^\beta$  and  $F^\beta$  for the  $\beta$ -shape.  $V^\beta$  consists of the centers of all atoms. Therefore,  $\beta$ -shape can be obtained from Voronoi diagram of atoms,  $VD(A)$  in  $O(|V^V| + |E^V| + |F^V|)$  time in the worst-case by looking into edges and faces of  $VD(A)$ . Fig. 1(c) shows the  $\beta$ -shape transformed from Voronoi diagram of atoms(Fig. 1(b)) and the molecular surface of the protein model in Fig. 1(a) based on the  $\beta$ -shape is shown in Fig. 1(d).

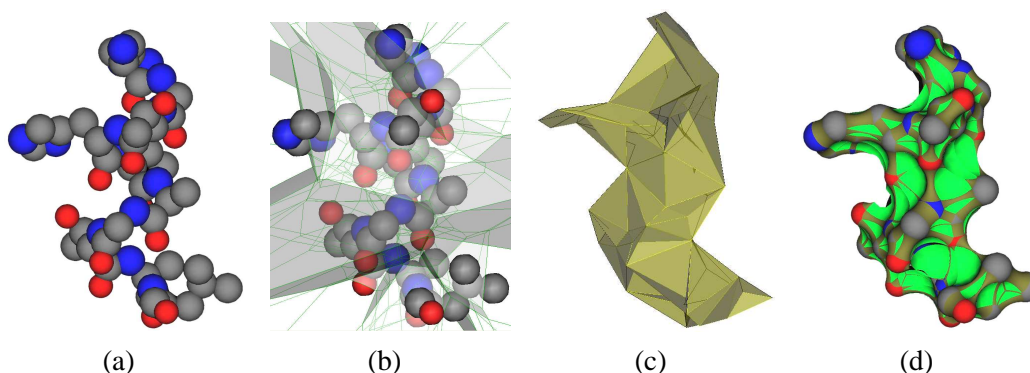


Figure 1. Molecular surface of atomic complex by  $\beta$ -shape based on Voronoi diagram of atoms. (a) atomic complex with 67 atoms, (b) the Voronoi diagram of atoms (c) the  $\beta$ -shape by a probe of radius  $1.4\text{\AA}$ , (d) the molecular surface corresponding to a probe of radius  $1.4\text{\AA}$

### REFERENCES

1. Connolly, Michael L., "Analytical molecular surface calculation", *Journal of Applied Crystallography*, Vol. 16, 1983, pp. 548-558.
2. Richards, Frederic M., "Areas, volumes, packing and protein structure", *Annu. Rev. Biophys. Bioeng.*, Vol. 6, 1977, pp. 151-176.
3. Varshney, A., Brooks FP Jr. and Richardson, David C., "Defining, Computing, and Visualizing Molecular Interfaces", *Proc. of 6th IEEE Visualization Conference*, pp 36-43, 1995.
4. Bajaj, Chandrajit L., Pascucci, V., Shamir A., Holt, Robert J. and Netravali, Arun N., "Dynamic maintenance and visualization of molecular surfaces", *Discrete Applied Mathematics*, Vol. 127, 2003, pp. 23-51.
5. Varshney, A., Brooks FP Jr., Wright, WV., "Computing Smooth Molecular Surfaces", *IEEE Computer Graphics and Applications*, Vol. 14, No. 5, 1994, pp. 19-25.
6. Kim, D.-S., Cho Y. and Kim D., "Euclidean Voronoi diagram of 3D balls and its computation via tracing edges", *Computer-Aided Design*, Vol. 37, No. 13, 2005, pp. 1412-1424.