

A β -complex for three-dimensional spheres

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ABSTRACT

In recent years, there have been extensive studies on biological systems such as proteins in various aspects. Being one of the important aspect, geometry is not the exception at all since the morphology mostly determines the functions of molecular systems. Hence, a strong driving force has been focused on the geometric aspect of such biological systems. Due to this consideration, the representation of proximity information among atoms(spheres) in the system has been one of the core research topics and the Voronoi diagram of atoms has been studied quite extensively in recent years[12,13].

By introducing the concept of α -shapes, Edelsbrunner and Mücke provided a basis for the applications of Voronoi diagram for a point set in reconstructing the shape from which the point set is produced[3]. They also provided very efficient codes to compute α -shapes using properties of Delaunay triangulation. Since α -shapes are fundamentally based on the rigorous theory of a Voronoi diagram of a point set and efficient and robust codes are available, α -shapes have been used in various applications. The main applications of α -shapes lie in the field of reasoning the surface shape which the point set defines. Based on this property, many researchers have tried to use it for reasoning the spatial structure of biological systems [4–7].

However, α -shapes have limitations in their applications in biological systems mainly due to the fact that α -shapes do not properly account for the size variations among atoms. In order to incorporate the size differences among the spheres, power diagrams have been used to more properly represent the topological relationship among them[1,2]. Power diagrams themselves also have limitations in various applications requiring measures of Euclidean distance metric since the power distance metric is used in their definition.

β -shape considers systematically size differences of the spheres and definition of a β -shape is identical to the definition of the well-known α -shape, proposed by Edelsbrunner and Mücke[3], except that the β -shape is based on spheres instead of points in a 3-dimension[8]. Recently, it has been shown that a β -shape is computationally convenient tool for various applications on three-dimensional spheres. For example, the recognition of pockets, the computation of molecular surfaces, etc. are all computed very efficiently using the β -shape of the atomic structure[14,9].

In this paper, we introduce the concept of β -complex which contains all of the possible β -shapes. Then, we present the algorithm to compute β -complex from the Voronoi diagram of spheres in $O(m \log m)$, where m is the number of simplices of the dual structure of Voronoi diagram. Once β -complex is obtained, a particular β -shape corresponding to a given β -value can be computed in $O(\log m + k)$ from the given β -complex, where k is the number of simplices

of β -shape.

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