Available online at www.sciencedirect.com
ScienceDirect
Computer-Aided Design 38 (2006) 1179–1191
COMPUTER-AIDED DESIGN
www.elsevier.com/locate/cad

Three-dimensional beta shapes

Deok-Soo Kim[a,b,*], Jeongyeon Seo[a], Donguk Kim[b], Joonghyun Ryu[b], Cheol-Hyung Cho[c]

[a] *Department of Industrial Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-gu, Seoul 133-791, South Korea*
[b] *Voronoi Diagram Research Center, Hanyang University, 17 Haengdang-dong, Seongdong-gu, Seoul 133-791, South Korea*
[c] *Corporate Technology Operations, Samsung Electronics Co., Ltd., 416 Maetan-3-dong, Yeongtong-gu, Suwon, Gyeonggi-do 443-742, South Korea*

Received 14 June 2005; accepted 21 July 2006

Abstract

The Voronoi diagram of a point set has been extensively used in various disciplines ever since it was first proposed. Its application realms have been even further extended to estimate the shape of point clouds when Edelsbrunner and Mücke introduced the concept of α-shape based on the Delaunay triangulation of a point set.

In this paper, we present the theory of β-shape for a set of three-dimensional spheres as the generalization of the well-known α-shape for a set of points. The proposed β-shape fully accounts for the size differences among spheres and therefore it is more appropriate for the efficient and correct solution for applications in biological systems such as proteins.

Once the Voronoi diagram of spheres is given, the corresponding β-shape can be efficiently constructed and various geometric computations on the sphere complex can be efficiently and correctly performed. It turns out that many important problems in biological systems such as proteins can be easily solved via the Voronoi diagram of atoms in proteins and β-shapes transformed from the Voronoi diagram.

Keywords: α-shape; α-hull; Weighted α-shape; β-shape; β-hull; Voronoi diagram; Delaunay triangulation

1. Introduction

The Voronoi diagram and its related concepts have been quite popular in various disciplines including science and engineering [1]. In particular, the Voronoi diagram for a point set has been increasingly used over the past several years for various applications. This is due to a greater understanding of its mathematical and computational properties as well as the development of robust yet efficient codes [1–3].

In biology, for example, the Voronoi diagram of the centers of atoms in a molecule was first used by Richards in 1974 to study the packing density of molecules [4]. Since then the Voronoi diagram has been used as one of the most important computational tools for the structure analysis for molecules.

Since 1974, the Voronoi diagram of a point set has been used quite extensively in the solution process of various structural biology problems. However, it was immediately noticed by Richards himself that the ordinary Voronoi diagram of points does not take the size variation among the atoms into account [4]. Richards, therefore, proposed to translate the planar bisector between two atoms in the Voronoi diagram according to the size difference between the two atoms. However, the translations of bisectors caused the so-called *vertex error* since this transformation does not guarantee a correct tessellation of the space in general [5]. In 1982, Gellatly and Finney proposed the use of a radical plane as the bisector between two atoms since the radical planes as bisectors guarantee no vertex error [5]. While reflecting the size variations among atoms at a certain level, this transformation guarantees a valid tessellation of the space. The tessellation using radical planes is indeed identical to the power diagram named by Aurenhammer [6].

By introducing the noble concept of α-shapes in 1994, Edelsbrunner and Mücke provided a basis for the applications of the Voronoi diagram of a point set in reconstructing the shape from which the point set is produced [7]. They also

* Corresponding author at: Department of Industrial Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-gu, Seoul 133-791, South Korea. Tel.: +82 2 2220 0472; fax: +82 2 2292 0472.
E-mail addresses: dskim@hanyang.ac.kr (D.-S. Kim), jyseo@voronoi.hanyang.ac.kr (J. Seo), donguk@voronoi.hanyang.ac.kr (D. Kim), jhryu@voronoi.hanyang.ac.kr (J. Ryu), murick.cho@samsung.com (C.-H. Cho).

0010-4485/$ - see front matter
doi:10.1016/j.cad.2006.07.002

provided an efficient code to compute α-shapes using properties of Delaunay triangulation. Since α-shapes are fundamentally based on the rigorous theory of the Voronoi diagram of a point set and the Delaunay triangulation, they have been used in various applications. The main applications of α-shapes lie in the field of reasoning the surface shape which a point set defines. Based on this property, many researchers have tried to use α-shapes for restructuring and reasoning the spatial structure of biological systems [8–11].

However, α-shapes have limitations in their applications in biological systems mainly due to the fact that α-shapes do not account for the size variation among atoms at all. In general, the proximity among spheres is not necessarily identical to the proximity among the centers of the spheres [12,13].

In order to incorporate the size difference among atoms, Edelsbrunner generalized the α-shape to the *weighted* α-shape using the regular triangulation which is the topological dual of the power diagram of the atoms [14,15]. Since then the weighted α-shapes have been used in the restructuring and reasoning of spatial structure for molecular systems [8–11]. However, weighted α-shapes themselves also have limitations in biological applications based on the Euclidean distance metric even though they reflect the size variations of atoms at a certain level.

In this paper, we present the theory of β-shape which reflects the size difference among spheres in their full Euclidean metric. Being the generalization of the α-shape in the Euclidean metric, the β-shape provides a complete consideration of the size differences among spheres. As will be elaborated in this paper, the proposed β-shape facilitates more convenient and powerful algorithms than the α-shape and the weighted α-shape for the applications based on the Euclidean distance. After the β-shape is defined, various properties of β-shapes including their similarities and dissimilarities with α-shapes are discussed. Then, the algorithm to compute β-shapes is presented based on the Voronoi diagram of spheres in the Euclidean distance metric. The proposed construct is called a β-shape since it is based on the concept of βlending over spheres. In addition, the name, β-shape, also implies that it is the generalization of the α-shape.

In Section 2, we provide a brief review of the well-known concepts of α-hull, α-shape and weighted α-shape. In Section 3, we present the need for another structure, β-shape, by illustrating the limitations of α-shape and weighted α-shape with a few examples. In Section 4, we present a motivation for the study of geometric problems in biological systems since we believe the CAD and CAGD community can find new opportunity in biology. In Sections 5 and 6, we introduce the concept of β-hull and β-shape and discuss a few properties of these new constructs. In Section 7, we present algorithms to construct β-shapes from the Voronoi diagram of spheres.

2. Reviews of α-family

In this section, we briefly review the three-dimensional α-shape and its weighted counterpart. Let S be a finite set of points in $\mathbb{R}^3$ and α satisfy $0 \leq \alpha \leq \infty$. The following paragraph, quoted from Edelsbrunner and Mücke [7], explains α-hulls and α-shapes very intuitively yet clearly.

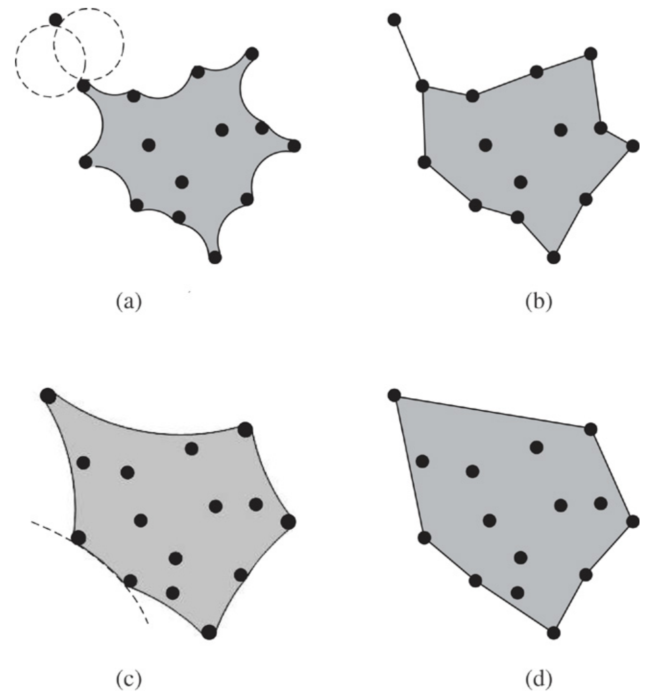

Fig. 1. Illustration of α-hulls and α-shapes for an identical point set in the plane. (a) An α-hull for α_1, (b) the corresponding α-shape for α_1, (c) an α-hull for α_2 where $\alpha_1 < \alpha_2$, and (d) the α-shape corresponding to α_2.

> "Think of $\mathbb{R}^3$ filled with Styrofoam and the points of S made of more solid material, such as rock. Now imagine a spherical eraser with radius α. It is omnipresent in the sense that it carves out Styrofoam at all positions where it does not enclose any of the sprinkled rocks, that is, points of S. The resulting object will be called the α-*hull*. To make things more feasible we straighten the surface of the object by substituting straight edges for the circular ones and triangles for the spherical caps. The obtained object is the α-*shape* of S."

Therefore, an α-shape is identical to the convex hull of S when $\alpha = \infty$. For $\alpha = 0$, the α-shape reduces to the point set S itself. In general, α-shapes can be concave and disconnected. α-shapes can contain two-dimensional patches of triangles and one-dimensional strings of edges. Its components can be even points. An α-shape is a subset of the closure of the Delaunay triangulation of S, and it may have handles and interior voids.

Let ∂X, $i(X)$, and $cl(X)$ denote the boundary, the interior, and the closure of a set X, respectively. In addition, let $\mathcal{H}_\alpha(S)$ and $\mathcal{S}_\alpha(S)$ denote an α-hull and an α-shape of the set S. Then, it can be shown that in general $\partial i(\mathcal{S}_\alpha(S)) \neq \partial\mathcal{S}_\alpha(S)$. This implies that α-shapes are non-manifold in general.

Fig. 1(a) shows a point set in the plane and an α-hull defined on the point set for a particular value of α_1. The corresponding α-shape for α_1 is shown in Fig. 1(b) with a dangling edge. Similarly, Fig. 1(c) and (d) illustrates the α-hull and α-shape of the same input points for α_2, respectively, where $0 < \alpha_1 < \alpha_2$. As shown in the figure, the α-hull for α_1 is a subset of the