Three-dimensional Alpha Shapes

Herbert Edelsbrunner Ernst P Mücke

Department of Computer Science
University of Illinois at Urbana-Champaign
1304 W Springfield Ave
Urbana, IL 61801

Abstract. *Frequently, data in scientific computing is in its abstract form a finite point set in space, and it is sometimes useful or required to compute what one might call the "shape" of the set. For that purpose this paper introduces the formal notion of the family of α-shapes of a finite point set in $\mathbb{R}^3$. Each shape is a polytope, derived from the Delaunay triangulation of the point set, with a parameter $\alpha \in \mathbb{R}$ controlling the desired level of detail. An algorithm is presented that constructs the entire family of shapes for a given set of size n in worst-case time $O(n^2)$. A robust implementation of the algorithm is discussed and several applications in the area of scientific computing are mentioned.*

1 Introduction

The geometric notion of "shape" has no associated formal meaning. This is in sharp contrast to other geometric notions, such as diameter, volume, convex hull, etc. The goal of this paper is to offer a concrete and formal definition of shape that can be computed and applied. It is not supposed to possibly cover the entire range of meanings the term "shape" carries in our contemporary language, even if restricted to geometric contexts. Nevertheless, it is sufficiently flexible to facilitate a wide range of applications including the study of molecular structures and the distribution of galaxies in our universe (section 7).

More specifically, the topic of this paper is the definition and computation of the shape of a finite point set in three-dimensional Euclidean space, $\mathbb{R}^3$. Intuitively, we think of the set as a cloud of points and we talk about the shape of this cloud. A peculiar aspect of the common usage of the word "shape" is that its meaning varies with the degree of detail intended. This aspect will be reflected by defining a one-parametric family of shapes ranging from "fine" and "local" to "crude" and "global".

A fair amount of related work has been done for point sets in $\mathbb{R}^2$, and some for point sets in $\mathbb{R}^3$. Jarvis [19] was one of the first to consider the problem of computing the shape as a generalization of the convex hull of a planar point set. A mathematically rigorous definition of shape was later introduced by Edelsbrunner, Kirkpatrick, and Seidel [10]. Their notion of α-shape is the two-dimensional analogue of the spatial notion described in this paper. Two-dimensional α-shapes are related to the dot patterns of Fairfield [13,14] and the circle diagrams used in bivariate cluster analysis, see eg, Moss [27]. Different graph structures that serve similar purposes are the Gabriel graph [26] and the relative neighborhood graph [32]. For $\mathbb{R}^3$, Boissonnat [1] suggested the use of Delaunay triangulations in connection with heuristics to "sculpture" a single connected shape of a point set. Our concept of shape is more general and mathematically well defined. Finally, we mention the superficial similarity between α-shapes and isosurfaces in $\mathbb{R}^3$. The latter is a popular concept in volume visualization, see eg, [6,24].

1992 Workshop on Volume Visualization/10/92/Boston, MA
© 1992 ACM 0-89791-528-3/92/0010/0075...$1.50

The outline of this paper is as follows. A formal definition of α-shapes, along with illustrations, is presented in section 2. Geometric concepts related to α-shapes are discussed in section 3. These are α-hulls, α-diagrams (also known as space-filling diagrams), α-complexes, and Delaunay triangulations. The result of a combinatorial analysis of α-shapes is stated in section 4. Using Delaunay triangulations, it is fairly easy to compute α-shapes in $\mathbb{R}^3$. The resulting algorithm is sketched in section 5. Given a set of n points in $\mathbb{R}^3$, it constructs a convenient implicit representation of the family of *all* α-shapes in time $O(n^2)$, worst case. This algorithm has been implemented by the second author of this paper. In section 6 we report on some aspects of the implementation, such as robustness and data structures. Section 7 discusses a few application problems that might benefit from the use of α-shapes. Finally, section 8 considers possible extensions of the material presented in this paper.

2 Alpha Shapes in Space

This section gives an intuitive description as well as a formal definition of three-dimensional α-shapes. Both are supported by illustrations that show point sets with sample members of their α-shape family. The beauty and elegance of the concept of an α-shape will hopefully be obvious after reading section 3 where relationships to other natural geometric concepts are revealed.

Intuitive Description. Conceptually, α-shapes are a generalization of the convex hull of a point set. Let S be a finite set in $\mathbb{R}^3$ and α a real number with $0 \leq \alpha \leq \infty$. The α-shape of S is a polytope that is neither necessarily convex nor necessarily connected. For $\alpha = \infty$, the α-shape is identical to the convex hull of S. However, as α decreases, the α-shape shrinks by gradually developing cavities. These cavities may join to form tunnels, and even holes may appear (see figure 1).[1]

Intuitively, a piece of the polytope disappears when α becomes small enough so that a sphere with radius α, or several such spheres, can occupy its space without enclosing any of the points of S. Think of $\mathbb{R}^3$ filled with Styrofoam and the points of S made

[1]The color plate of figure 1 shows six different shapes for a set with points randomly generated on the surface of two linked tori. The first shape is the convex hull, for $\alpha = +\infty$, the last shape is the point set itself, for $\alpha = 0$. The α-value used in the forth frame neatly separates the two tori. Further decreasing α disassembles the shape. Singular triangles are shown in darker color.

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 (section 3). To make things more feasible we straighten the object's surface by substituting straight edges for the circular ones and triangles for the spherical caps. The thus obtained object is the α-shape of S (see figure 2).[2] It is a polytope in a fairly general sense: it can be concave and even disconnected, it can contain two-dimensional patches of triangles and one-dimensional strings of edges, and its components can be as small as single points. The parameter α controls the maximum "curvature" of any cavity of the polytope.

General Position. Throughout this paper we assume that the points of S are in general position. For the time being, this means that no 4 points lie on a common plane, no 5 points lie on a common sphere, and for any fixed α, the smallest sphere through any 2, 3, or 4 points of S has a radius different from α. The general position assumption will later be extended when convenient (section 5.3). It simplifies forthcoming definitions, discussions, and algorithms, and is justified by a programming technique, known as SoS [11]. This method simulates an infinitesimal perturbation of the points on the level of geometric predicates and relieves the programmer from the otherwise necessary case analysis (section 6.1).

Formal Definition. For $0 < \alpha < \infty$, let an *α-ball* be an open ball with radius α. For completeness, a *0-ball* is a point and an *∞-ball* is an open half-space. An α-ball b is *empty* if $b \cap S = \emptyset$. Any subset $T \subseteq S$ of size $|T| = k+1$, with $0 \le k \le 3$, defines a *k-simplex* Δ_T that is the convex hull of T, also denoted by $\text{conv}(T)$. The general position assumption assures that all k-simplices are properly k-dimensional. For $0 \le k \le 2$, such a k-simplex Δ_T is said to be *α-exposed* if there is an empty α-ball b with $T = \partial b \cap S$, where ∂b is the sphere or plane bounding b. A fixed α thus defines sets $F_{k,\alpha}$ of α-exposed k-simplices, for $0 \le k \le 2$. The *α-shape* of S, denoted by $\mathcal{S}_\alpha$, is the polytope whose boundary consists of the triangles in $F_{2,\alpha}$, the edges in $F_{1,\alpha}$, and the vertices in $F_{0,\alpha}$ (see figures 1 and 2). The k-simplices in $F_{k,\alpha}$ are also called the *k-faces* of $\mathcal{S}_\alpha$.

We still need to specify which connected components of $\mathbb{R}^3 - \partial\mathcal{S}_\alpha$ are interior and which are exterior to $\mathcal{S}_\alpha$. Fix the value of α and notice that for each α-exposed triangle Δ_T there are two (not necessarily empty) α-balls, $b_1 \neq b_2$, so that $T \subseteq \partial b_1$ and $T \subseteq \partial b_2$. If both α-balls are empty then Δ_T does not belong to the boundary of the interior of $\mathcal{S}_\alpha$. Otherwise, assume that b_1 is empty and that b_2 is not. In this case, Δ_T bounds the interior of $\mathcal{S}_\alpha$. More specifically, the interior of $\mathcal{S}_\alpha$ and the center of b_1 lie on different sides of Δ_T. The definition of interior and exterior of $\mathcal{S}_\alpha$ is possibly more natural in the context of Delaunay triangulations and α-complexes described in section 3.

[2] The color plate of figure 2 shows six shapes of a set based on demo data for Silicon Graphics' Solidview program, of course, without any of the original connectivity information. The erasing sphere is shown to the right of the shape. Apart from a dense conglomerate of points representing part of the person's brain, the set is basically hollow with most points representing skin.

3 Related Geometric Concepts

There are quite a few natural geometric concepts that are closely related to α-shapes. Some of them are discussed in this section. In each case, the emphasis is on how the concept is related to α-shapes and how this relation can enrich our understanding of α-shapes. Section 3.1 discusses α-hulls and α-diagrams. Section 3.2 briefly reviews Delaunay triangulations. The relevance of the Delaunay triangulation of a point set is that each α-shape of the set is the underlying space of a subcomplex of the triangulation. These subcomplexes are termed α-complexes and defined in section 3.3. Extensions of these notions are mentioned in section 3.4.

3.1 Alpha Hulls and Alpha Diagrams

Recall from section 2 that for positive real α an α-ball is defined as an open ball with radius α. For $\alpha = 0$ it is a point and for $\alpha = \infty$ it is an open half-space. Given a finite point set $S \subseteq \mathbb{R}^3$, an α-ball is empty if $b \cap S = \emptyset$. For $0 \le \alpha \le \infty$, the *α-hull* of S, denoted by $\mathcal{H}_\alpha$, is defined as the complement of the union of all empty α-balls. This is the formal counterpart of the Styrofoam object described in section 2. Sample members of the continuous family of α-hulls are the convex hull of S, for $\alpha = \infty$, and S itself, for α sufficiently small. Observe that $\mathcal{H}_{\alpha_1} \subseteq \mathcal{H}_{\alpha_2}$ if $\alpha_1 \le \alpha_2$.

Another interesting concept defined by α-balls is what we call the *α-diagram* of S, denoted by $\mathcal{F}_\alpha$. For $0 < \alpha < \infty$, $\mathcal{F}_\alpha$ is the union of all α-balls whose centers are points in S.[3] Observe that a point $x \in \mathbb{R}^3$ belongs to $\mathcal{F}_\alpha$ iff the α-ball centered at x is not empty. Denote this α-ball by b_x. This implies the following close relationship between $\mathcal{H}_\alpha$ and $\mathcal{F}_\alpha$.

$$x \in \mathcal{F}_\alpha \iff b_x \cap \mathcal{H}_\alpha \neq \emptyset, \text{ and}$$
$$x \in \mathcal{H}_\alpha \iff b_x \subseteq \mathcal{F}_\alpha.$$

Although α-hulls and α-diagrams are interesting geometric concepts, they are not important for the developments in this paper. Further details are thus omitted.

3.2 Delaunay Triangulations

A finite point set $S \subseteq \mathbb{R}^3$ defines a special triangulation known as the Delaunay triangulation of S, see eg, [8,28]. Assuming general position of the points, this triangulation is unique and decomposes the convex hull of S into tetrahedra.

For $0 \le k \le 3$, let F_k be the set of k-simplices $\Delta_T = \text{conv}(T)$, $T \subseteq S$ and $|T| = k+1$, for which there are empty open balls b with $\partial b \cap S = T$. Notice that $F_0 = S$. The *Delaunay triangulation* of S, denoted by $\mathcal{D}$, is the cell complex defined by the tetrahedra in F_3, the triangles in F_2, the edges in F_1, and the vertices in F_0. By definition, for each simplex $\Delta_T \in \mathcal{D}$, there exist values of $\alpha \ge 0$ so that Δ_T is α-exposed. Conversely, every face of $\mathcal{S}_\alpha$ is a simplex of $\mathcal{D}$. This implies the following relationship between the Delaunay triangulation and the boundary of $\mathcal{S}_\alpha$.

$$F_k = \bigcup_{0 \le \alpha \le \infty} F_{k,\alpha}, \text{ for } 0 \le k \le 2.$$

We take advantage of this relationship by representing the family of α-shapes of S implicitly by the Delaunay triangulation of S. This will be described in detail in section 5.

[3] In chemistry and biology, α-diagrams are known as space-filling diagrams. However, there they are usually not restricted to equally large balls. This restriction can be removed with weighted α-shapes and α-diagrams (section 3.4).

3.3 Alpha Complexes

Since all faces of $\mathcal{S}_\alpha$ are simplices of $\mathcal{D}$, it follows that the interior of $\mathcal{S}_\alpha$ is naturally triangulated by the tetrahedra of $\mathcal{D}$. This idea leads to the concept of α-complexes as defined shortly. A (three-dimensional) *simplicial cell complex* is a collection $\mathcal{C}$ of closed k-simplices, for $0 \leq k \leq 3$, that satisfies the following two properties.

(i) If $\Delta_T \in \mathcal{C}$ then $\Delta_{T'} \in \mathcal{C}$ for every $T' \subseteq T$. In other words, with every simplex Δ_T, $\mathcal{C}$ contains all faces of Δ_T as well.

(ii) If $\Delta_T, \Delta_{T'} \in \mathcal{C}$ then either $\Delta_T \cap \Delta_{T'} = \emptyset$ or $\Delta_T \cap \Delta_{T'} = \Delta_{T \cap T'} = \text{conv}(T \cap T')$. Note that (i) implies that this face is also in $\mathcal{C}$. In other words, the intersection of any two simplices in $\mathcal{C}$ is either empty or a face of both.

A subset $\mathcal{C}' \subseteq \mathcal{C}$ is a *subcomplex* of $\mathcal{C}$ if it is also a simplicial cell complex.

Each k-simplex Δ_T of $\mathcal{D}$ defines an open ball b_T bounded by the smallest sphere that contains T. Let ϱ_T be the radius of b_T. For $k = 3$, ∂b_T is the circumsphere of Δ_T, for $k = 2$, the circumcircle of Δ_T is a great circle of ∂b_T, and for $k = 1$, the two points in T are antipodal on ∂b_T. Call ∂b_T the *smallest circumsphere* and ϱ_T the *radius* of Δ_T. For $1 \leq k \leq 3$ and $0 \leq \alpha \leq \infty$, define $G_{k,\alpha}$ as the set of k-simplices $\Delta_T \in \mathcal{D}$ for which b_T is empty and $\varrho_T < \alpha$. Furthermore, define $G_{0,\alpha} = S$, for all α. The sets $G_{k,\alpha}$ do not necessarily define a cell complex because it can happen that $G_{3,\alpha}$ contains a tetrahedron but not all triangles of this tetrahedron belong to $G_{2,\alpha}$. Similarly for triangles and edges. With this in mind, we define the *α-complex* of S, denoted by $\mathcal{C}_\alpha$, as the cell complex whose k-simplices are either in $G_{k,\alpha}$ or they bound $(k+1)$-simplices of $\mathcal{C}_\alpha$. By definition, $\mathcal{C}_{\alpha_1}$ is a subcomplex of $\mathcal{C}_{\alpha_2}$ if $\alpha_1 \leq \alpha_2$.

The *underlying space* of $\mathcal{C}_\alpha$, denoted by $|\mathcal{C}_\alpha|$, is the union of all simplices of $\mathcal{C}_\alpha$, or in other words, the part of $\mathbb{R}^3$ covered by $\mathcal{C}_\alpha$. Thus, the underlying space of $\mathcal{C}_\alpha$ is a polytope in the sense specified in section 2. Indeed, we have the following most important property of $\mathcal{C}_\alpha$, which we present without proof.

For all $0 \leq \alpha \leq \infty$, $\mathcal{S}_\alpha = |\mathcal{C}_\alpha|$.

This can be considered an alternative definition of α-shapes.

3.4 Extensions

The definitions presented in sections 2 and 3 above can be extended in various ways. So far we refrained from mentioning these extensions in order to avoid unnecessary complications and to be faithful to the currently available implementation of the concepts in this paper. For completeness, some of these are now briefly discussed.

Weighted Points. Recall the relationship between α-shapes and α-diagrams described in section 3.1. It is interesting to consider diagrams for different ball sizes, and this is indeed done in chemistry and biology where space-filling diagrams are usually defined as unions of balls with arbitrary and thus possibly different radii. In order to represent such diagrams by polytopes similar to α-shapes it is necessary to introduce weighted α-shapes. These can be defined using subcomplexes of so-called regular triangulations, see eg, [9, 23]. Given a finite set of points, each with a real weight, the regular triangulation is a unique cell complex whose underlying space is the convex hull of the point set. If all weights are the same then it is exactly the Delaunay triangulation of the points. Details of weighted α-shapes will be studied elsewhere.

Higher Dimensions. It is fairly straightforward to generalize all important concepts of this section (ie, α-shapes, α-hulls, α-diagrams, α-complexes, and Delaunay triangulations) to finite point sets S in $\mathbb{R}^d$, for arbitrary d. Of course, implementation details need to be changed accordingly, and, in general, the complexity of the algorithms increases exponentially with d. For example, if S is a set of n points in $\mathbb{R}^d$ then the Delaunay triangulation of S can consist of up to $\Theta(n^{\lfloor \frac{d+1}{2} \rfloor})$ faces, see, eg, [31]. Although the running time of the programs constructing α-shapes will get substantially worse as d increases, there might be applications that warrant the implementation of α-shapes in dimensions that are small but larger than three.

4 Combinatorial Analysis

The α-shapes of a finite point set form a discrete family, even though they are defined for *all* real numbers α, with $0 \leq \alpha \leq \infty$. Indeed, $\mathcal{S}_{\alpha_1} \neq \mathcal{S}_{\alpha_2}$ iff $\bigcup_{k=0}^{3} G_{k,\alpha_1} \neq \bigcup_{k=0}^{3} G_{k,\alpha_2}$. Thus, $\mathcal{S}_{\alpha_1} \neq \mathcal{S}_{\alpha_2}$ iff there is an empty open ball bounded by a smallest circumsphere of an edge, triangle, or tetrahedron of $\mathcal{D}$ whose radius lies between α_1 and α_2. Such a radius is referred to as an *α-threshold* because it separates two α-shapes. The number of α-shapes exceeds the number of α-thresholds by one. It follows that one plus the total number of k-simplices of $\mathcal{D}$, for $1 \leq k \leq 3$, is an upper bound on the number of different α-shapes. A bound on this number can be obtained by lifting Delaunay triangulations in $\mathbb{R}^3$ to convex polytopes in $\mathbb{R}^4$, see, eg, [8]. The upper bound theorem for convex polytopes implies bounds on the number of faces in terms of n, the number of vertices. This leads to the following result which we state without further details.

S has at most $2n^2 - 5n$ different α-shapes. (4-1)

5 Algorithms

As described in section 3, the family of α-shapes of a finite point set S can be represented by the Delaunay triangulation of S. In this representation, each simplex of $\mathcal{D}$ is associated with an interval that specifies for which values of α the simplex belongs to the α-shape. Section 5.1 gives references for the construction of $\mathcal{D}$, and section 5.2 explains how the intervals of the simplices are computed. For completeness, section 5.3 gives the formulas that can be used to implement the required primitive operations.

5.1 Three-dimensional Delaunay Triangulations

The construction of Delaunay triangulations is a popular topic in the area of geometric algorithms [8, 28]. Indeed, various different approaches have been studied and described in the literature. Some approaches are based on the lifting map, mentioned in section 4, which transforms the problem into one of constructing the convex hull of a four-dimensional point set.

The algorithm adopted for our implementation of α-shapes has been suggested by Joe [20]. It is based on the idea of local transformations or flips.[4] The algorithm can be viewed as a generaliza-

[4] As recently shown, the flip algorithm can be extended to compute regular triangulations in arbitrary dimensions [12]. Regular triangulations are useful for weighted α-shapes (section 3.4).

tion of the edge-flip method for two-dimensional triangulations by Lawson [22]. Unfortunately, the straightforward generalization of the two-dimensional algorithm to $\mathbb{R}^3$ fails to always compute the Delaunay triangulation. Nevertheless, the correctness of the flip algorithm in $\mathbb{R}^3$ can be established if the points are added in an incremental fashion, see [21].

5.2 Intervals and Face Classification

For each simplex $\Delta_T \in \mathcal{D}$ there is a single interval so that Δ_T is a face of the α-shape $\mathcal{S}_\alpha$ iff α is contained in this interval. It will be convenient to study these intervals for the α-complex $\mathcal{C}_\alpha$ rather than the α-shape. We also break each interval into three (possibly empty) parts that correspond to values of α for which the simplex is an interior, regular, or singular simplex of $\mathcal{C}_\alpha$.

A simplex $\Delta_T \in \mathcal{C}_\alpha$ is said to be

$$\begin{cases} \textit{interior} & \text{if } \Delta_T \notin \partial\mathcal{S}_\alpha, \\ \textit{regular} & \text{if } \Delta_T \in \partial\mathcal{S}_\alpha \text{ and it bounds some} \\ & \text{higher-dimensional simplex in } \mathcal{C}_\alpha, \text{ and} \\ \textit{singular} & \text{if } \Delta_T \in \partial\mathcal{S}_\alpha \text{ and it does not bound} \\ & \text{any higher-dimensional simplex in } \mathcal{C}_\alpha. \end{cases}$$

Notice that there are Delaunay edges and triangles that can never be singular because their smallest circumsphere encloses other points of S.[5] Therefore, we call a simplex $\Delta_T \in \mathcal{D}$

$$\begin{cases} \textit{attached} & \text{if } |T| = 2,3 \text{ and } b_T \cap S \neq \emptyset, \text{ and} \\ \textit{unattached} & \text{otherwise.} \end{cases}$$

Recall that ϱ_T is the radius of the smallest circumsphere of Δ_T. For a simplex $\Delta_{T'} \in \mathcal{D}$, $|T| \leq 3$, let $\mathrm{up}(\Delta_T)$ be the set of all simplices in $\mathcal{D}$ that contain Δ_T as a proper face, that is, $\mathrm{up}(\Delta_T) = \{\Delta_{T'} \in \mathcal{D} \mid T \subset T'\}$. If Δ_T is a tetrahedron, define $\underline{\mu}_T = \overline{\mu}_T = \varrho_T$. Otherwise,

$$\underline{\mu}_T = \min\{\varrho_{T'} \mid \Delta_{T'} \in \mathrm{up}(\Delta_T), \text{ unattached}\} \text{ and}$$
$$\overline{\mu}_T = \max\{\varrho_{T'} \mid \Delta_{T'} \in \mathrm{up}(\Delta_T)\}.$$

It is sufficient to consider only the set

$$\mathrm{up}_1(\Delta_T) = \{\Delta_{T'} \in \mathrm{up}(\Delta_T) \mid |T'| = |T| + 1\},$$

that is, all faces incident to Δ_T whose dimension is one higher than that of Δ_T, in order to derive the values $\underline{\mu}_T$ and $\overline{\mu}_T$:

$$\underline{\mu}_T = \min \begin{pmatrix} \{\varrho_{T'} \mid \Delta_{T'} \in \mathrm{up}_1(\Delta_T), \text{ unattached}\} \\ \cup \;\; \{\underline{\mu}_{T'} \mid \Delta_{T'} \in \mathrm{up}_1(\Delta_T), \text{ attached}\} \end{pmatrix},$$

and

$$\overline{\mu}_T = \max\{\overline{\mu}_{T'} \mid \Delta_{T'} \in \mathrm{up}_1(\Delta_T)\}.$$

Specifying Intervals. The intervals of α values in which Δ_T is an interior, regular, or singular simplex of $\mathcal{C}_\alpha$ are shown in the table 1. Because of the general position assumption, α is different from all ϱ values and therefore also from all $\underline{\mu}$ and $\overline{\mu}$ values. We can thus define all intervals as open, except at endpoints 0 and ∞. It is necessary to distinguish simplices that bound the convex hull of S from the others. The next paragraph briefly explains the entries of table 1 for the case of triangles that do not bound the convex hull of S. The arguments for tetrahedra, triangles on the convex hull, edges, and vertices are similar.

[5] It is convenient to extend the general position assumption so that no smallest circumsphere of two or three points of S contains another point of S. A slightly more general assumption is the following. If a sphere contains three points of S then no two of them are antipodal, and if it contains four points then no three lie on a great-circle of the sphere.

		singular	regular	interior
tetrahedron				$(\varrho_T, \infty]$
edge or triangle,	$\notin \partial\mathrm{conv}(S)$, unattached	$(\varrho_T, \underline{\mu}_T)$	$(\underline{\mu}_T, \overline{\mu}_T)$	$(\overline{\mu}_T, \infty]$
	$\notin \partial\mathrm{conv}(S)$, attached		$(\underline{\mu}_T, \overline{\mu}_T)$	$(\overline{\mu}_T, \infty]$
	$\in \partial\mathrm{conv}(S)$, unattached	$(\varrho_T, \underline{\mu}_T)$	$(\underline{\mu}_T, \infty]$	
	$\in \partial\mathrm{conv}(S)$, attached		$(\underline{\mu}_T, \infty]$	
vertex,		$[0, \underline{\mu}_T)$	$(\underline{\mu}_T, \overline{\mu}_T)$	$(\overline{\mu}_T, \infty]$
	$\in \partial\mathrm{conv}(S)$	$[0, \underline{\mu}_T)$	$(\underline{\mu}_T, \infty]$	

Table 1: Intervals of α values for which $\Delta_T \in \mathcal{D}$ belongs $\mathcal{C}_\alpha$.

Consider a triangle $\Delta_T \in \mathcal{D}$, $T = \{p_i, p_j, p_k\}$, that does not bound the convex hull of S; we denote this by $\Delta_T \notin \partial\mathrm{conv}(S)$. Let $\Delta_{T'}$ and $\Delta_{T''}$ be the two incident tetrahedra in $\mathcal{D}$, and assume $T' = T \cup \{p_u\}$, and $T'' = T \cup \{p_v\}$. Furthermore, be $\varrho_{T'} < \varrho_{T''}$, in other words, $\underline{\mu}_T = \varrho_{T'}$ and $\overline{\mu}_T = \varrho_{T''}$. Now, fix a value for α. If $\varrho_{T''} < \alpha \leq \infty$, then the triangle Δ_T is not α-exposed; it will, however, be part of the interior of $\mathcal{S}_\alpha$, because both incident tetrahedra are in $\mathcal{C}_\alpha$. If $\varrho_{T'} < \alpha < \varrho_{T''}$, then the triangle is α-exposed and $\Delta_{T'}$ is in $\mathcal{C}_\alpha$ but $\Delta_{T''}$ is not. This means that $\Delta_{T'}$ is a regular triangle of $\mathcal{C}_\alpha$. When $\alpha < \varrho_{T'}$, neither $\Delta_{T'}$ nor $\Delta_{T''}$ are tetrahedra of $\mathcal{S}_\alpha$, but Δ_T can still be a singular triangle, that is, iff $\varrho_T < \alpha$ and neither p_u nor p_v are inside b_T. If one apex is inside b_T, then Δ_T is attached. That is, it can never be a singular triangle of $\mathcal{C}_\alpha$, no matter what α value is selected.

The α-complex consists of all interior, regular, and singular simplices for a given α value. The interior of the α-shape is triangulated by the interior simplices. The boundary of the interior is formed by the set of regular triangles and their edges and vertices.

Consistent with the definition in section 4, we refer to the endpoints of the intervals in table 1 as α-thresholds. This does not include 0 and ∞. Since all $\underline{\mu}_T$ and $\overline{\mu}_T$ values are ϱ values of other simplices, each α-threshold is the radius of a simplex in $\mathcal{D}$. More specifically, the set of α-thresholds is exactly the set of radii of all unattached k-simplices, for $1 \leq k \leq 3$. Define the ***α-spectrum*** as the sorted sequence of α-thresholds. This concept will appear again in section 6.

Computing Intervals. Assume, that each simplex $\Delta_T \in \mathcal{D}$ is marked as either "$\in \partial\mathrm{conv}(S)$" or "$\notin \partial\mathrm{conv}(S)$" after the construction of $\mathcal{D}$. With this, the above intervals can be computed by classifying Δ_T as attached or unattached, and by computing ϱ_T, $\underline{\mu}_T$, and $\overline{\mu}_T$, whenever applicable. We said that Δ_T is attached iff one of the simplices that contain Δ_T has a vertex in b_T, the open ball bounded by the smallest circumsphere of Δ_T. This implies that Δ_T can be classified in time proportional to $|\mathrm{up}_1(\Delta_T)|$. The time it takes to classify *all* simplices is proportional to the number of simplices in $\mathcal{D}$, because each simplex has only a constant number of faces. In other words, assuming that constant time suffices to decide whether or not a point belongs to b_T (see section 5.3), a simplex can be classified in constant amortized time.

Furthermore, assume that, given T with $\Delta_T \in \mathcal{D}$, ϱ_T can be computed in constant time (again, see section 5.3). By processing tetrahedra before triangles before edges before vertices, we can get $\underline{\mu}_T$ and $\overline{\mu}_T$ simply as the minimum and maximum of the values $\varrho_{T'}$, $\underline{\mu}_{T'}$, and $\overline{\mu}_{T'}$, for $\Delta_{T'} \in \mathrm{up}_1(\Delta_T)$. This also takes only constant amortized time per simplex.

5.3 Geometric Primitives

What are the primitive operations needed to compute α-shapes in $\mathbb{R}^3$? Constructing the Delaunay triangulations requires two geometric tests. These are a test for deciding on which side of a plane spanned by three points a fourth point lies, and one for deciding on which side of a sphere spanned by four points a fifth point lies. In order to generate the intervals of table 1, we need to compute the radius of the smallest circumsphere of a tetrahedron, triangle, or edge, and test whether a point lies inside or outside this sphere. While the two tests required for Delaunay triangulations are fairly common in geometric algorithms and computer graphics, the operations involving smallest circumspheres of triangles and edges are rather specialized. All operations share the problem of degenerate cases, which we can ignore because of the general position assumption (see also section 6). This section gives a formula for each of the primitive operations mentioned above.

Assume that the points of S are labeled as $p_1, p_2, \ldots, p_n$, and that each point p_i is given by the vector $(\pi_{i,1}, \pi_{i,2}, \pi_{i,3})$ of its three coordinates. To simplify the notation in the remainder of this section, we use minors, which are determinants of submatrices of a given matrix. For convenience, define $\pi_{i,0} = 1$ for all i and use the following notation for minors:

$$\mathcal{M}^{i_1,i_2,\ldots,i_k}_{j_1,j_2,\ldots,j_k} = \det \begin{pmatrix} \pi_{i_1,j_1} & \pi_{i_1,j_2} & \cdots & \pi_{i_1,j_k} \\ \pi_{i_2,j_1} & \pi_{i_2,j_2} & \cdots & \pi_{i_2,j_k} \\ \vdots & \vdots & \ddots & \vdots \\ \pi_{i_k,j_1} & \pi_{i_k,j_2} & \cdots & \pi_{i_k,j_k} \end{pmatrix}.$$

Plane Test. Let $T = \{p_i, p_j, p_k\}$ and define h_T as the unique plane that contains all three points of T. This plane can be oriented if we replace the *set* T by the *sequence* T, eg, $T = (p_i, p_j, p_k)$. Then one side (or open half-space) of h_T can be called *positive* and the other *negative*. We also refer to these as the positive and negative sides of the sequence (p_i, p_j, p_k).

$$p_u \text{ lies on the } \textit{positive} \text{ side of } h_T \iff \mathcal{M}^{i,j,k,u}_{1,2,3,0} > 0, \qquad (5\text{-}1)$$

and p_u lies on the *negative* side if the determinant is negative. Intuitively, p_u sees the sequence of three points p_i, p_j, p_k in a clockwise order iff p_u lies on their positive side. Similarly, p_u sees the sequence in a counterclockwise order iff p_u lies on the negative side of the points. The sign of the determinant is called the *orientation* of the sequence (p_i, p_j, p_k, p_u). Notice that the determinant equals zero iff the points are in degenerate position, that is, they lie on a common plane. Observe also that the orientation of a permutation of a sequence of four points is the same as the orientation of the sequence itself, provided the number of transpositions is even. Otherwise, it is the opposite. This follows trivially from the fact that the value of the determinant changes sign whenever two rows are exchanged.

Sphere Test. Given a set $T = \{p_i, p_j, p_k, p_u\}$, we need to decide whether another point p_v lies inside or outside the sphere ∂b_T. We can assume that the degererate case where $p_v \in \partial b_T$ does not occur. A possible implementation of this test is discussed in [11] using an extension of the lifting map, mentioned in section 4, to three-dimensional spheres. Let U: $x_4 = \sum_{\ell=1}^{3} x_\ell^2$ be a paraboloid in $\mathbb{R}^4$. A sphere ∂b with center $c = (\gamma_1, \gamma_2, \gamma_3)$ and radius ρ is mapped to the hyperplane ∂b_U: $x_4 = \sum_{\ell=1}^{3}(2\gamma_\ell x_\ell - \gamma_\ell^2) + \rho^2$. This hyperplane has the property that $U \cap \partial b_U$ projected along the x_4-axis into the $x_1x_2x_3$-space yields ∂b. Moreover, a point p lies inside (outside) ∂b iff p_U lies vertically below (above) ∂b_U. The resulting formula assumes that each point $p_i \in S$ has a fourth coordinate $\pi_{i,4} = \sum_{j=1}^{3} \pi_{i,j}^2$.

$$p_v \text{ lies inside } \partial b_T \iff \mathcal{M}^{i,j,k,u}_{1,2,3,0} \cdot \mathcal{M}^{i,j,k,u,v}_{1,2,3,4,0} > 0 \qquad (5\text{-}2)$$

The first minor, $\mathcal{M}^{i,j,k,u}_{1,2,3,0}$, is a corrective term that is necessary because the sphere does not change if the first four points are permuted. The second minor, $\mathcal{M}^{i,j,k,u,v}_{1,2,3,4,0}$, expresses the fact that the lifting map transforms a sphere test in $\mathbb{R}^3$ to a hyperplane test in $\mathbb{R}^4$.

Radius of a Smallest Circumsphere. Next, we consider computing the radius ϱ_T of ∂b_T, the smallest circumsphere of Δ_T, for all k-simplices $\Delta_T \in \mathcal{D}$, with $1 \le k \le 3$. The formulas for the square of ϱ_T are given in (5-3) through (5-5). Note that computing ϱ_T^2 will be sufficient for our purposes since ϱ_T can never be negative. We distinguish the cases when $k = |T| - 1$ is 1, 2, or 3.

$T = \{p_i, p_j\}$:

$$\varrho_T^2 = \frac{\left(\mathcal{M}^{i,j}_{1,0}\right)^2 + \left(\mathcal{M}^{i,j}_{2,0}\right)^2 + \left(\mathcal{M}^{i,j}_{3,0}\right)^2}{4} \qquad (5\text{-}3)$$

$T = \{p_i, p_j, p_k\}$:

$$\varrho_T^2 = \frac{\left(\sum_{\ell=1}^{3}\left(\mathcal{M}^{i,j}_{\ell,0}\right)^2\right) \cdot \left(\sum_{\ell=1}^{3}\left(\mathcal{M}^{j,k}_{\ell,0}\right)^2\right) \cdot \left(\sum_{\ell=1}^{3}\left(\mathcal{M}^{k,i}_{\ell,0}\right)^2\right)}{4 \cdot \left(\left(\mathcal{M}^{i,j,k}_{2,3,0}\right)^2 + \left(\mathcal{M}^{i,j,k}_{1,3,0}\right)^2 + \left(\mathcal{M}^{i,j,k}_{1,2,0}\right)^2\right)} \qquad (5\text{-}4)$$

$T = \{p_i, p_j, p_k, p_u\}$:

$$\varrho_T^2 = \frac{\left(\mathcal{M}^{i,j,k,u}_{2,3,4,0}\right)^2 + \left(\mathcal{M}^{i,j,k,u}_{1,3,4,0}\right)^2 + \left(\mathcal{M}^{i,j,k,u}_{1,2,4,0}\right)^2}{4 \cdot \left(\mathcal{M}^{i,j,k,u}_{1,2,3,0}\right)^2} + \frac{\mathcal{M}^{i,j,k,u}_{1,2,3,0} \cdot \mathcal{M}^{i,j,k,u}_{1,2,3,4}}{\left(\mathcal{M}^{i,j,k,u}_{1,2,3,0}\right)^2} \qquad (5\text{-}5)$$

In order to explain these three formulas we introduce some notation. Let a, b, c, d be points in $\mathbb{R}^3$. We write $|ab|$ for the *length* of the edge $\mathrm{conv}(\{a, b\})$, and $|abc|$ for the *area* of the triangle $\mathrm{conv}(\{a, b, c\})$. In the case of two points, ϱ_T is the same as half the distance between p_i and p_j. Equation (5-3) follows because

$$|p_i p_j|^2 = \left(\mathcal{M}^{i,j}_{1,0}\right)^2 + \left(\mathcal{M}^{i,j}_{2,0}\right)^2 + \left(\mathcal{M}^{i,j}_{3,0}\right)^2.$$

To handle the case of a triangle, ie, $T = \{p_i, p_j, p_k\}$, we use the formulas

$$\varrho_T = \frac{|p_i p_j| \cdot |p_j p_k| \cdot |p_k p_i|}{4 \cdot |p_i p_j p_k|} \quad \text{and}$$

$$|p_i p_j p_k|^2 = \frac{1}{4} \cdot \left(\left(\mathcal{M}^{i,j,k}_{2,3,0}\right)^2 + \left(\mathcal{M}^{i,j,k}_{1,3,0}\right)^2 + \left(\mathcal{M}^{i,j,k}_{1,2,0}\right)^2\right)$$

which can be found in any good mathematical handbook. Finally, we obtain (5-5) using the extension of the lifting map mentioned above. If ∂b is the sphere through points p_i, p_j, p_k, p_u then ∂b_U is the hyperplane through the four points $p_{i,U}, p_{j,U}, p_{k,U}, p_{u,U}$. The equation for the hyperplane can be computed directly from the coordinates of the lifted points. From this equation it is easy to compute the center and the radius of ∂b.

Attached and Unattached Edges and Triangles. We still have to consider the problem of deciding whether an edge or triangle $\Delta_T \in \mathcal{D}$ is attached or not. By definition, Δ_T is attached if there is a $\Delta_R \in \mathrm{up}_1(\Delta_T)$ so that the point in $R - T$ belongs to b_T. If Δ_T is an edge, say, $T = \{p_i, p_j\}$ and $R - T = \{p_k\}$, this can be done by comparing ϱ_T with the distance between p_k and $\frac{p_i + p_j}{2}$. Straightforward algebraic manipulations lead to the following equation.

$$p_k \in b_T \iff \sum_{\ell=1}^{3}\left(\mathcal{M}^{i,j}_{\ell,0}\right)^2 - \sum_{\ell=1}^{3}\left(\mathcal{M}^{i,k}_{\ell,0} + \mathcal{M}^{j,k}_{\ell,0}\right)^2 > 0 \qquad (5\text{-}6)$$

Now let Δ_T be a triangle, eg, $T = \{p_i, p_j, p_k\}$ and $R - T = \{p_u\}$.

To see whether or not the point p_u belongs to b_T, we compute the center c of the circumsphere ∂b_R of the tetrahedron Δ_R. Observe that $p_u \in b_T$ iff c and p_u do not lie on the same side of the plane through p_i, p_j, p_k. In other words, we need to test whether or not the sequences (p_u, p_i, p_j, p_k) and (c, p_i, p_j, p_k) have different orientation. Some rather tedious algebraic manipulations are needed to derive the following equation which expresses the derivation in terms of minors.

$$p_u \in b_T \iff \begin{cases} \mathcal{M}^{i,j,k,u}_{2,3,4,0} \cdot \mathcal{M}^{i,j,k}_{2,3,0} + \mathcal{M}^{i,j,k,u}_{1,3,4,0} \cdot \mathcal{M}^{i,j,k}_{1,3,0} \\ + \mathcal{M}^{i,j,k,u}_{1,2,4,0} \cdot \mathcal{M}^{i,j,k}_{1,2,0} - 2 \cdot \mathcal{M}^{i,j,k,u}_{1,2,3,0} \cdot \mathcal{M}^{i,j,k}_{1,2,3} \\ > 0 \end{cases} \tag{5-7}$$

General Position Revisited. The general position assumption used in this paper assures that no geometric test is ambiguous. We summarize and revise the necessary assumptions below and include pointers to the formulas for which the assumptions are relevant.

- No 4 points lie on a common plane; cf (5-1).
- No 5 points lie on a common sphere; cf (5-2).
- No smallest circumsphere of 2, 3, or 4 points has a radius equal to any given α; cf (5-3)–(5-5).
- No point lies on the smallest circumsphere of 2 or 3 other points; cf (5-6) and (5-7).

These assumptions are indeed very restrictive and rarely true for real-life data. We will deal with this apparent shortcoming in section 6.1.

6 Implementation

Our current implementation of a software tool for α-shapes in $\mathbb{R}^3$ consists of the following three parts.

1. A program that constructs Delaunay triangulations using flips (section 5.1).
2. A program that computes the intervals for all simplices in a Delaunay triangulation, and then sorts the enpoints of these intervals (section 5.2).
3. An α-shape visualizer that enables the user to manually select different α values and render the corresponding shape on a graphics workstation (figures 1 through 6).

Parts 1 and 2 are preprocessing steps that take time $O(n^2)$ and $O(m \log m)$, where n is the number of points and m is the number of simplices of $\mathcal{D}$. The current code for part 3 takes time $O(m)$ to render a particular α-shape. Improvements based on fast data structures for intervals are forthcoming.

6.1 Simulated Perturbation

For implementation purposes it is no longer appropriate to assume that the input points are in general position. This assumption would be too restrictive. On the other hand, in the context of three-dimensional α-shapes, it would be rather tedious to deal with the large number of special cases in an ad-hoc manner. For this reason, we apply a general technique, known as Simulation of Simplicity or SoS [11], which acts as a black box between the implementation of a geometric algorithm and the input data. It allows a systematic treatment of all special cases on the level of geometric primitive operations. The SoS library consists of a set of carefully implemented primitives. It provides the programmer with the illusion of simple data while the actual input is in arbitrary and thus possibly degenerate position.[6] Refer to [11] for details.

6.2 Data Structures

There are two main data structures needed for storing the family of α-shapes of a given data set. One represents the connectivity and order among the simplices of the three-dimensional Delaunay triangulations. The other is used for the intervals assigned to the simplices of $\mathcal{D}$. A triangle-based data structure is used to store $\mathcal{D}$. This is briefly described in the paragraphs below. An interval tree can be used to store the collection of intervals, see eg, [28]. The current version of our program, however, only stores the α-spectrum using a linear array. Recall that the α-spectrum is the sorted sequence of α-thresholds. Universal hashing, see eg, [4], provides the link between the triangle structure and the array.

The data structure used to store the three-dimensional triangulation is a specialized version of the edge-facet structure introduced by Dobkin and Laszlo [5]. Related data structures are the quad-edge structure due to Guibas and Stolfi [18], which can be used to model two-dimensional manifolds, and the cell-tuple structure by Brisson [2], which works in arbitrary dimensions. The edge-facet structure is designed for general cell complexes in three dimensions. By reducing the scope to triangulations, it is possible to improve the compactness and the speed of the structure. We refer to the result as the *triangle-edge structure*.

The atomic unit of the triangle-edge structure is the so-called *triangle-edge pair* $a = \langle \Delta, i \rangle$, with $0 \le i \le 5$. It identifies six versions of the triangle Δ, one for each of its six directed edges. Each triangle defines two *edge rings*. One edge ring traverses the edges of Δ in a counterclockwise order, the other traverses them in a clockwise order. Similarly, each edge defines two *triangle rings* traversing the incident triangles in the two opposite orders. Each triangle-edge a belongs to exactly one edge ring and exactly one triangle ring.

The internal representation of the structure takes advantage of the fact that all edge rings have length three. It is thus possible to avoid actual pointers for the edge rings by merging the six triangle-edge pairs of two opposite edge rings into one record. Such a record allocates 30 (36) bytes per triangle, assuming that 2-byte (4-byte) integers are used as indices to the vertices, and 4-byte integers for triangle-edge pairs. Further details are omitted.

7 Applications and Further Illustrations

It is important to point out that α-shapes are a fairly generic tool that can be used in many applications that have to do with shape, including automatic mesh generation and geometric modeling (see

[6] The terms "simple," "general position," and "nondegenerate position" are used as synonyms. Notice how the "general case" of the algorithm designer is usually the "simple case" for the implementing programmer.

figures 3 and 4).[7] Indeed, they can be used as a concrete expression of shape, which is often all that is needed. Similarly, three-dimensional α-shapes can be used to identify clusters in trivariate data. Beyond these generic applications, there are others that rely on particular properties of α-shapes. For these applications, it would be difficult to replace α-shapes by any other reasonable notion of shape. Two such applications are briefly addressed below.

Molecular Structures. Molecules are usually modeled as conglomerates of atoms with fixed relative positions. Each atom is represented by a ball around a center point, and the radius of the ball depends on what the model is supposed to express. For example, in the so-called space-filling diagram (section 3.1) the balls encompass the idealized locations of the electrons so that balls of nearby atoms typically overlap. This diagram, defined as a union of balls, is in a strict geometric sense dual to the α-shape of the center points, assuming each ball has radius equal to α. The α-shape can thus be used to compute structural and metric properties of the space-filling diagram, such as its connectivity, surface area, or volume. Alternatively, the α-shape itself, for this value of α, can be used to model and manipulate the molecule. When different atoms are represented by balls of *different* sizes then weighted α-shapes need to be used (section 3.4).

Molecules with intersting α-shapes arise in the study of proteins and how they fold (see figure 5).[8] The geometric locations of the atoms of about 500 proteins are known today. However, there are many more gene sequences that can be determined. One of the goals of theoretical molecular biology is to obtain three-dimensional positional information from the knowledge of these sequences. This is the problem of protein folding [16,29]. Since the α-shape is computationally inexpensive and because it closely reflects the physical reality of molecules, it is hoped that α-shapes prove to be a useful tool in future protein folding research.

Distribution of a Point Set. An interesting though ill-defined geometric problem arises in the study of the distribution of galaxies in our universe. As observed in studies like in [3,15], the galaxies are distributed in an unexpected and rather nonuniform manner (see figure 6).[9] Astronomers have measured the location of about 170,000 galaxies, each one represented by a point in three-dimensional space. It appears that a large number of galaxies are located on or close to sheet-like and to filament-shaped structures. In other words, large subsets of the points are distributed in a predominantly two- or one-dimensional manner. How can this intuitive notion of the dimension of a point distribution be captured? A possible answer can be given by considering the entire family of α-shapes. Let $A(\alpha)$ be the surface area of the α-shape and let $V(\alpha)$ be its volume. It might be interesting to study the relative variation of A and V over the range of α values between 0 and ∞. In particular, the ratio $q(\alpha) = \frac{A(\alpha)}{V(\alpha)+1}$ might be worthwhile considering. Follow q as α decreases starting at ∞. If the point set is two-dimensionally distributed, one could observe that $V(\alpha)$ vanishes relative early while $A(\alpha)$ is still large. The ratio will reflect this behavior by an early spike. Other functions, possibly including the total edge length of the α-shape, can be used to quantify properties of point distributions that are otherwise difficult to capture. Such quantifications can be useful in the comparative study of the actually observed galaxy distribution and simulated data; see [7] for first steps in this direction. This kind of approach needs efficient algorithms that compute signature functions, such as A, V, and q (see section 8).

8 Summary and Open Problems

The main contribution of this paper is the introduction of a sound framework that formally captures the rather intuitive notion of the "shape" of a point set in space. This is the concept of three-dimensional α-shapes. A prototype version of a robust α-shape tool has been implemented. The authors of this paper hope that this tool will find many users within the engineering and the scientific computing and visualization communities. However, there is still a lot of work to be done. For example, the extensions mentioned in section 3.4 are worthwhile implementing, and this is planned in the near future. The extensions mentioned below are either less specific or theoretically not well understood.

Improving the Running Time. A large fraction of the time used to construct α-shapes is needed for computing the Delaunay triangulation of the points. The algorithm used in our implementation takes time $O(n^2)$ in the worst case, independent of the number of simplices of $\mathcal{D}$. However, it rarely exhibits worst-case behavior. Still, it would be useful to have an algorithm whose running time is linear in the size of $\mathcal{D}$. Is it possible to construct $\mathcal{D}$ in time $O(n \log n + m)$, where $m = |F_1 \cup F_2 \cup F_3|$? A first step towards such an algorithm is the output-sensitive convex hull algorithm of Seidel [30]. If combined with the methods of [25] it runs in time $O(n^{4/3+\varepsilon} + m \log n)$ for n points in $\mathbb{R}^3$. On a different level, the running time of our program can be improved by speeding up the geometric primitives which all reduce to integer computations (see section 6). According to our experimental studies, about 80% of the time is spent doing integer arithmetic. This implies that appropriate hardware support might have a significant impact on the running time.

Maintaining Alpha Shapes. In some applications it is necessary to construct α-shapes across a number of different point sets, and often these point sets are very similar to each other. For example, a point set might undergo local changes within an iterative process, and the α-shape or some feature of it is to be constructed at each step of the iteration. A local change might be the insertion of a new point, the deletion of an old point, the dislocation of one point, the dislocation of a subset of the points, etc. The development of efficient update algorithms that reuse available structure as much as possible can lead to dramatic improvements of the overall running time.

[7] The point sets to the color plates of figures 3 and 4 are based on demo data for modeling and rendering programs. All connectivity information of the modeling data, ie, edges and triangles, was removed, leaving only the vertex coordinates. As described in section 3, each α-shape is triangulated by the tetrahedra of the corresponding α-complex. This might be useful in the automatic generation of meshes for objects with nonconvex surfaces.

[8] The data to figure 5 represents a time-averaged molecular dynamics structure of gramicidin A, a peptide that forms a channel for ion and water movement across lipid membranes. The major structural motif is a right-handed beta-bonded helix. The tunnel of the macro-structure can be detected using relatively large α values. Smaller values of α result in shapes with larger numbers of isolated triangles and edges. These α-shapes reveal the helix of the micro-structure.

[9] The data in figure 6 represents a simulation of the positions of galaxies within our universe. The theory is that galaxies first clustered into sheet-like structures, then progressed to filament-shaped structures at the intersection of multiple sheets. As filaments began to intersect, global clusters appeared. It is interesting to investigate the macro- and micro-structure of the galaxies, including the detection of large voids and local or global clusters. The full spectrum of α-shapes promises to be useful in this study.

Features and Signatures. Individual α-shapes are interesting geometric objects, and it would be useful to have efficient algorithms that can analyze its geometric and topological properties or features. For example, computing the volume is fairly straightforward because the α-complex provides a triangulation of the α-shape, and the volume of the α-shape is simply the sum of the volumes of the tetrahedra. More challenging is the computation of the connectivity of the α-shape as expressed by its first three homology groups, see, eg, Giblin [17].

As suggested by the second application discussed in section 7, the history of a feature, over all values of α from 0 through ∞, is of interest. Consider some specific feature, say, the number of connected components of the α-shape. The corresponding ***signature*** is a function c: $[0, +\infty] \rightarrow \mathbb{R}$, so that $c(\alpha)$ is the number of components of $\mathcal{S}_\alpha$. This function reflects the evaluation of the number of components as α changes continuously from 0 to $+\infty$. Given the α-spectrum, it is fairly easy to compute c. Start at $\alpha = 0$ and maintain a union-find data structure, see, eg, [4], storing the components as threshold values are processed in increasing order. A more challenging task is the computation of the signatures for higher-order homology groups. Such signatures might be handy in the selection of an appropriate α value which typically depends on the application and the user's momentary focus of attention. With the current α-shape tool, α values are selected from the α-spectrum which is typically too large to be very effective.

Acknowledgements

Research of both authors is supported by the National Science Foundation under grant CCR-8921421. Work by the first author is also supported by the Alan T Waterman award, grant CCR-9118874. We thank Ping Fu, for her interest in the α-shape tool and her active encouragement and collaboration. We are also indebted to Marc Dyksterhouse, Eric Jakobson, Patrick Moran, Michael Norman, and Shankar Subramanian from NCSA for their valuable comments and interest in our work, and the staff at the NCSA Renaissance Experimental Lab for granting us access to their graphics workstations. The second author owes Donald Hearn from the CS Department at UIUC for triggering his interest in implementing an α-shape tool with a course on scientific visualization.

"Don't look like a convex hull... get yourself in α-shape!"
— David Knapp.

References

[1] J D Boissonnat. Geometric structures for three-dimensional shape representation. *ACM Transactions on Graphics*, 3(4):266–286, 1984.

[2] E Brisson. Representing geometric structures in d dimensions: topology and order. In *Proceedings of the 5th Annual Symposium on Computational Geometry*, pages 218–227, 1989.

[3] R Y Cen, A Jameson, F Liu, and J P Ostriker. The universe in a box: thermal effects in a standard cold dark matter scenario. *Astrophysical Journal (Letters)*, 362:L41, October 1990.

[4] T H Cormen, C E Leiserson, and R L Rivest. *Introduction to Algorithms*. MIT Press, Cambridge, Massachusetts, 1990.

[5] D P Dobkin and M J Laszlo. Primitives for the manipulation of three-dimensional subdivisions. *Algorithmica*, 4(1):3–32, 1989.

[6] R A Drebin, L Carpenter, and P Hanrahan. Volume rendering. *Computer Graphics*, 22(4):65–74, 1988. ACM Siggraph '88. Conference Proceedings.

[7] M D Dyksterhouse. An alpha-shape view of our universe. MS thesis, Department of Computer Science, University of Illinois at Urbana-Champaign, 1992.

[8] H Edelsbrunner. *Algorithms in Combinatorial Geometry*. Springer-Verlag, Heidelberg, Germany, 1987.

[9] H Edelsbrunner. Geometric algorithms. To appear in P Gruber and J Wills, editors, *Handbook of Convex Geometry*, North-Holland, 1992.

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

[11] H Edelsbrunner and E P Mücke. Simulation of Simplicity: a technique to cope with degenerate cases in geometric algorithms. *ACM Transactions on Graphics*, 9(1):66–104, 1990.

[12] H Edelsbrunner and N R Shah. Incremental topological flipping works for regular triangulations. In *Proceedings of the 8th Annual Symposium on Computational Geometry*, pages 43–52, 1992.

[13] J Fairfield. Contoured shape generation: forms that people see in dot patterns. In *Proceedings of the IEEE Conference on Cybernetics and Society*, pages 60–64, 1979.

[14] J Fairfield. Segmenting dot patterns by Voronoi diagram concavity. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 5(1):104–110, 1983.

[15] M J Geller and J P Huchra. Mapping the universe. *Science*, 246:897–903, November 1989.

[16] Ch Ghélis and J Yon. *Protein Folding*. Academic Press, 1982.

[17] P J Giblin. *Graphs, Surfaces, and Homology*. Second edition. Chapman and Hall, London, 1981.

[18] L J Guibas and J Stolfi. Primitives for manipulation of general subdivisions and the computation of Voronoi diagrams. *ACM Transactions on Graphics*, 4(2):74–123, 1985.

[19] R A Jarvis. Computing the shape hull of points in the plane. In *Proceedings of the IEEE Computing Society Conference on Pattern Recognition and Image Processing*, pages 231–241, 1977.

[20] B Joe. Construction of three-dimensional Delaunay triangulations using local transformations. *Computer Aided Geometric Design*, 8(2):123–142, 1991.

[21] B Joe. Three-dimensional triangulations from local transformations. *SIAM Journal on Scientific and Statistical Computing*, 10(4):718–741, 1989.

[22] C L Lawson. Software for C^1 surface interpolation. In J R Rice, editor, *Mathematical Software III*, pages 161–194, Academic Press, New York, 1977.

[23] C Lee. Regular triangulations of convex polytopes. In P Gritzmann and B Sturmfels, editors, *Applied Geometry and Discrete Mathematics: The Victor Klee Festschrift*, pages 443–456, American Mathematical Society, Providence, RI, 1991.

[24] W E Lorensen and H E Cline. Marching cubes: a high resolution 3D surface construction algorithm. *Computer Graphics*, 21(4):163–169, 1987. ACM Siggraph '87. Conference Proceedings.

[25] J Matoušek and O Schwarzkopf. Linear optimization queries. In *Proceedings of the 8th Annual Symposium on Computational Geometry*, pages 16–25, 1992.

[26] D W Matula and R R Sokal. Properties of Gabriel graphs relevant to geographic variation research and the clustering of points in the plane. *Geographical Analysis*, 12(3):205–222, 1980.

[27] W W Moss. Some new analytic and graphic approaches to numerical taxonomy, with an example from the Dermanyssidae (Acari). *Systematic Zoology*, 16:177–207, 1967.

[28] F P Preparata and M I Shamos. *Computational Geometry — An Introduction*. Springer-Verlag, New York, 1985.

[29] F M Richards. The protein folding problem. *Scientific American*, 264(1):54–63, 1991.

[30] R Seidel. Constructing higher-dimensional convex hulls in logarithmic cost per face. In *Proceedings of the 18th Annual ACM Symposium on Theory of Computing*, pages 484–507, Berkeley, California, 1986.

[31] R Seidel. Exact upper bounds for the number of faces in d-dimensional Voronoi diagrams. In P Gritzmann and B Sturmfels, editors, *Applied Geometry and Discrete Mathematics: The Victor Klee Festschrift*, pages 517–530, American Mathematical Society, Providence, RI, 1991.

[32] G T Toussaint. The relative neighborhood graph of a finite planar set. *Pattern Recognition*, 12(4):261–268, 1980.