

Computing Delaunay Triangulation and Alpha shape of a Protein Complex

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Introduction:

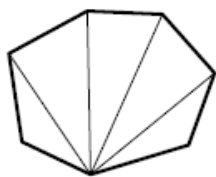
Protein structure determines protein function is a fundamental problem in molecular biology. We can use Computational Geometry to study the geometry, shape, physicochemical texture of binding surfaces to understand how they work and how functional roles of proteins can be predicted.

Computational Geometry is also used in the study of Protein-Protein, Protein-DNA, Protein-ligand Interactions and Protein Structure analysis.

In this study we will focus on Delaunay triangulation and Alpha shape.

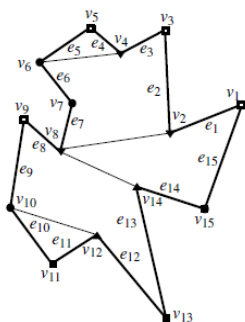
Basics of Triangulation:

Decomposition of a polygon into triangles by a maximal set of non-intersecting diagonals is called a Triangulation of the polygon. Polygon can be convex and non-convex. Convex polygon are easy to triangulate. We just pick one vertex and draw diagonals to all other vertices except the neighboring vertices.



Photograph from Computational Geometry Algorithms and Applications Book

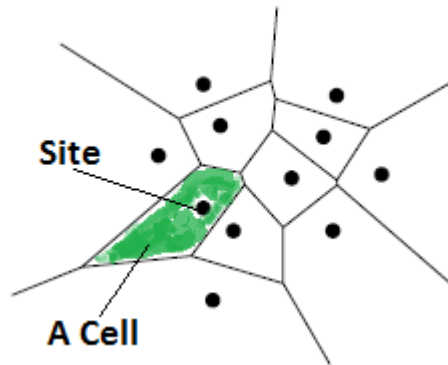
But for non-convex polygon this is not the case. (An approach to triangulate a non-convex polygon would be to first decompose it into convex pieces and then triangulate the pieces, but it is difficult to portion a polygon into convex pieces. So we first decompose the non-convex polygon into monotone pieces and then triangulate it)



Photograph from Computational Geometry Algorithms and Applications Book

Voronoi Diagram:

A simple voronoi diagram looks like below



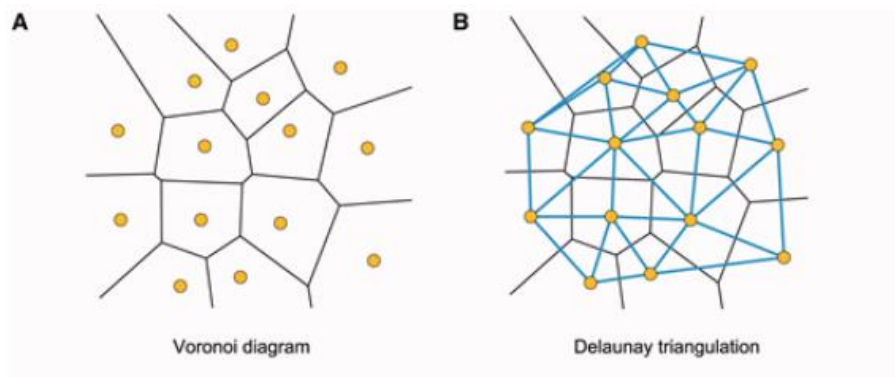
Voronoi diagram is obtained by partitioning of a plane with n points into convex polygons such that each polygon contains exactly one site and every point in the cell is closer to its site than to any other site.

The vertices of the diagram are Voronoi vertices and the line segments are Voronoi edges.

Each cell is formed by the common intersection of a number of half-planes. A voronoi diagram is a planar subdivision. Some edges are line segments and others are half-planes (a straight line extending from a point indefinitely in one direction only). Thales's theorem help us identify to see if an edge is legal or illegal. Half plane intersection method takes $O(n^2 \log n)$ times to construct the voronoi diagram, while fortune algorithm takes $O(n \log n)$ time.

Delaunay Triangulation:

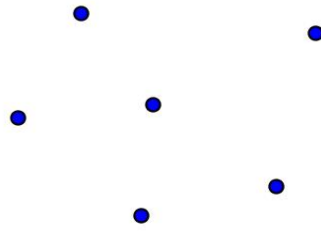
Dual graph of voronoi diagram is the Delaunay triangulation which is obtained by connecting the sites if the corresponding cells share the same edge.



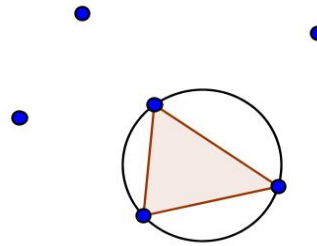
Photograph from <https://academic.oup.com/bib/article/15/1/54/187726>

The exterior face of the Delaunay Triangulation is the convex hull of the point set.

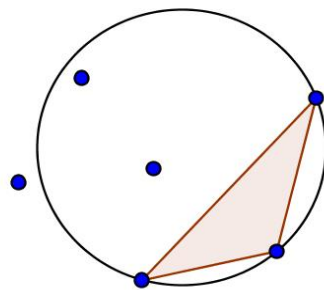
Empty circle Property: Also in Delaunay triangle every circumcircle of a triangle is an empty circle (means it does not contain a point of P in its interiors). The circumcircle of a triangle is the unique circle passing through the three vertices of the triangle



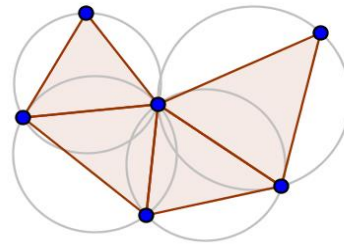
A collection of points



A Delaunay triangle



A non-Delaunay triangle



A Delaunay triangulation

Photograph from Google Images

Delaunay Triangulation contains vertices, Edges, Triangles and Tetrahedrons

- Vertices – 0 Simplex
- Edges – 1 Simplex
- Triangles – 2 Simplex
- Tetrahedrons – 3 Simplex

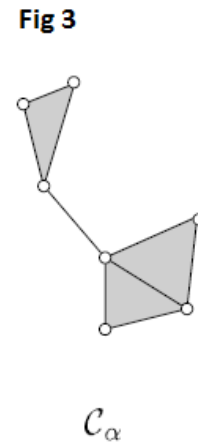
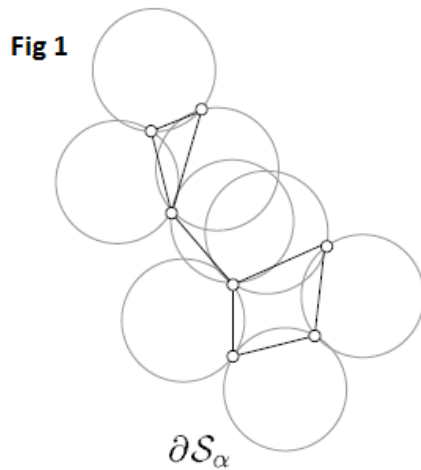
A k -simplex is a k -dimensional polytope which is the convex hull of its $k + 1$ vertices.

Alpha Complexes: To compute alpha shape

The alpha-complex of S is a sub complex of this triangulation of S , containing the alpha-exposed k -simplexes. A simplex is said to be alpha-exposed, if there is an open disk of radius $\sqrt{\alpha}$ through the vertices of the simplex that does not contain any other point of S .

Boundary: The boundary $\partial\mathcal{S}_\alpha$ of the α -shape of the point set S consists of all k -simplices of S for $0 \leq k < d$ which are α -exposed,

$$\partial\mathcal{S}_\alpha = \{\Delta_T \mid T \subset S, |T| \leq d \text{ and } \Delta_T \text{ } \alpha\text{-exposed}\}.$$



Photograph from Stanford School Website

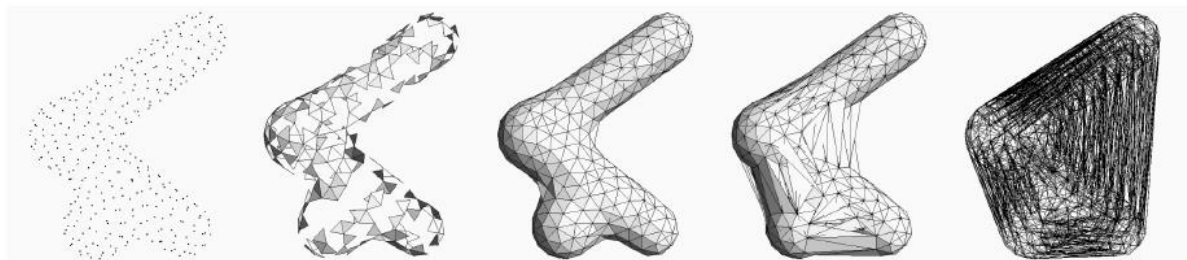
Fig 1 – Boundary of the alpha shape

Fig 2 – Delaunay Triangulation

Fig 3 – Alpha complex

From the figure we can see Alpha complex gives rise to Alpha shape. In Molecular Biology each atom is represented by a ball whose radius reflects the range of its van der Waals interactions and thus depends on the atom type.

How should we choose alpha value?



Photograph from Stanford School Website

All alpha shapes don't give good approximation about the object surface as you can see in this picture.

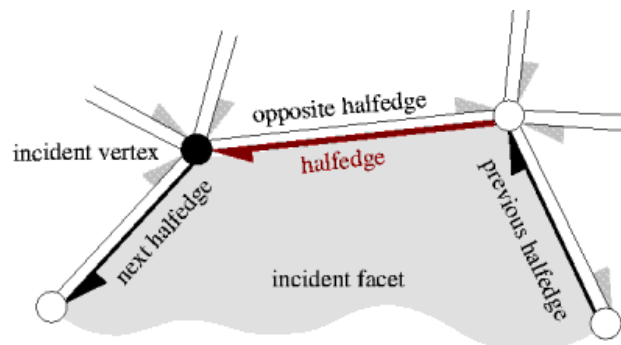
We can't choose alpha value to be too small and too large as alpha shapes are calculated based in distance between points in order to decide which points to connect by triangles or lines. One way to choose Optimum alpha value is by Trial and Error method.

Methods:

Used C++ CGAL library to compute the Delaunay Triangulation and Alpha shape

Filtration of Delaunay edges, facets and tetrahedra are done through alpha ball.

Vertices, Edges and triangles are stored in a half-edge (Doubly connected edge list) data structure.

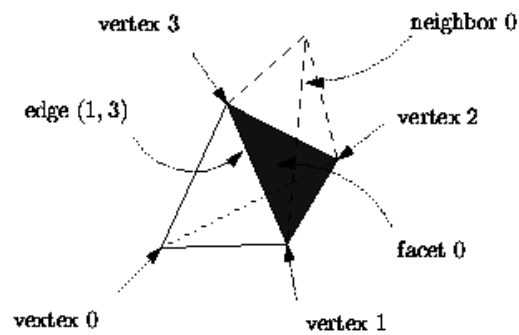


Half edge data structure

Photograph from CGAL Website

3D Triangulation Data Structure:

Each cell gives access to its four incident vertices and to its four adjacent cells. Each vertex gives direct access to one of its incident cells, which is sufficient to retrieve all the incident cells when needed. The four vertices of a cell are indexed with 0, 1, 2 and 3. The neighbors of a cell are also indexed with 0, 1, 2, 3 in such a way that the neighbor indexed by "i" is opposite to the vertex with the same index.



Photograph from CGAL Website

Delaunay Triangulation and Alpha shape Implementation:

Data Set: 2omz (Crystal structure of InlA Y369A/hEC1 complex)

Tools: Visual Studio 2012, MeshLab 3D

Library: CGAL (Computational Geometry Algorithms Library)

Language: C++

Details extracted from Delaunay Triangulation:

No of Finite Vertices – 5440

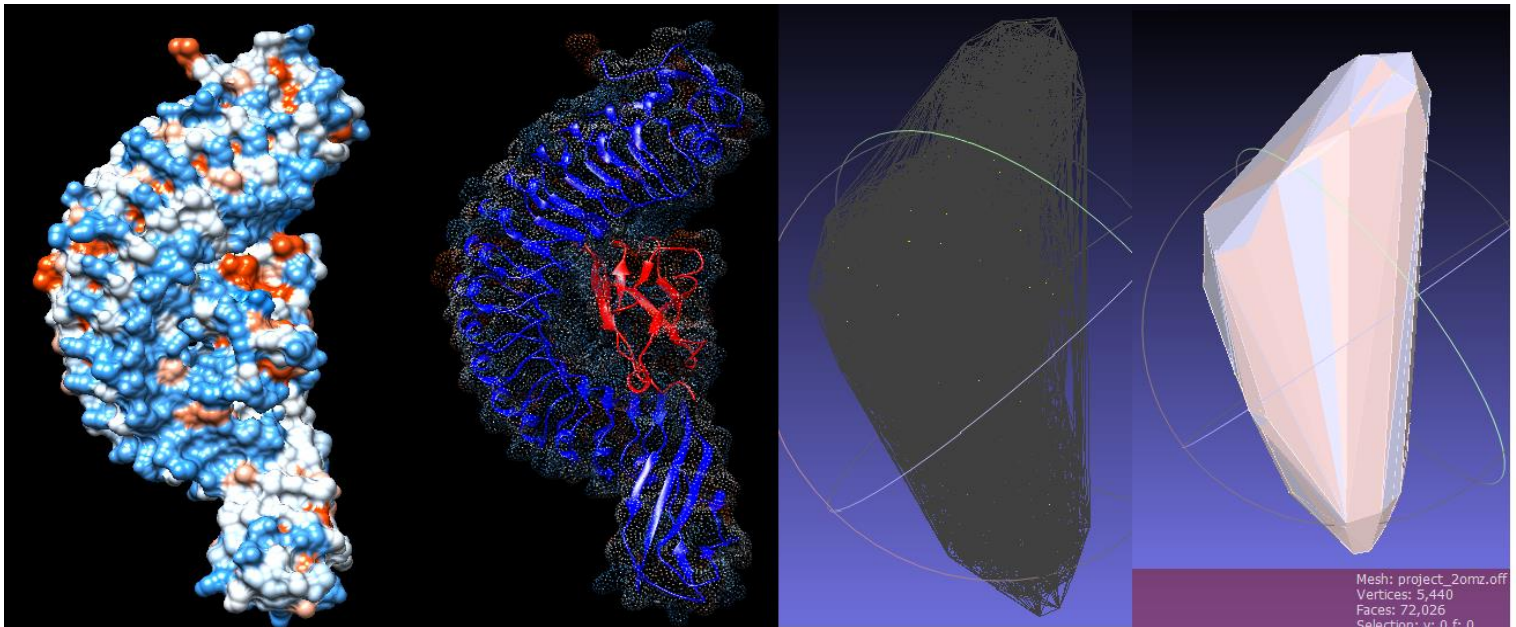
No of Finite Edges – 41500

No of Finite Faces – 72026

No of Finite Cells – 35965

Output File Format: OFF Files Geomview Object File Format

Delaunay Triangulation of 2omz:

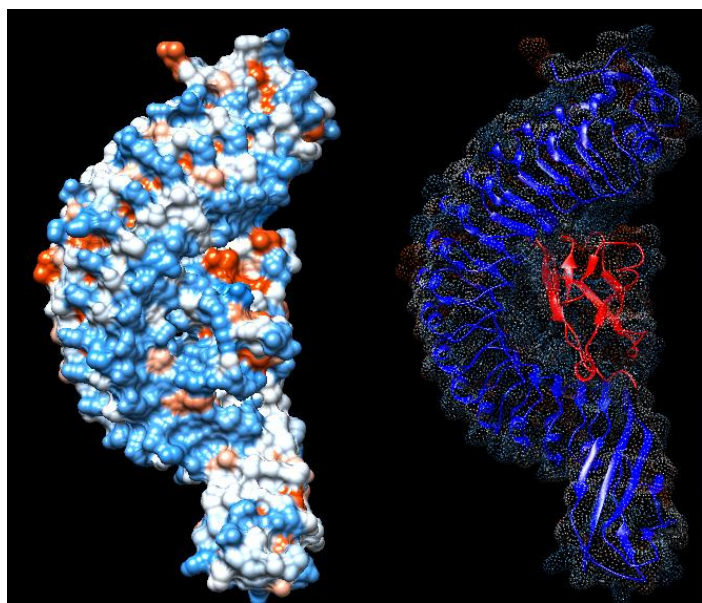


2omz in Chimera

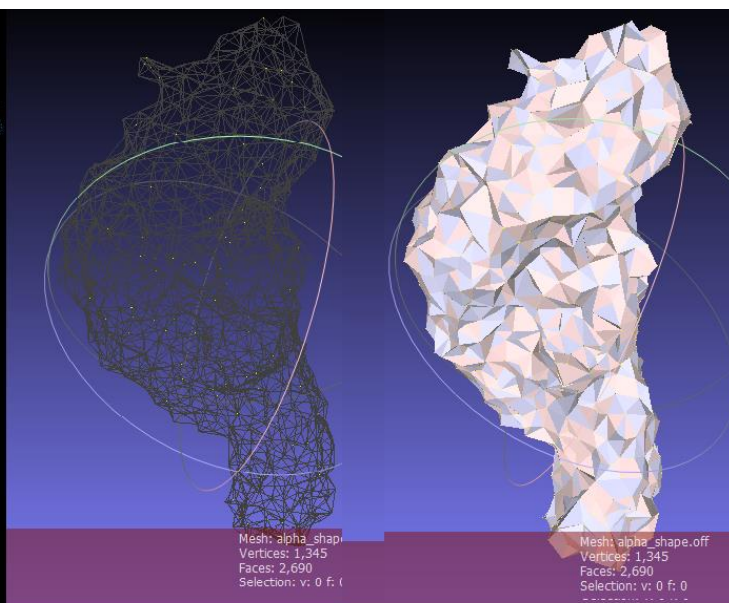
2omz DT in MeshLab

Alpha Shape of 2omz:

Using alpha value = 14.3215



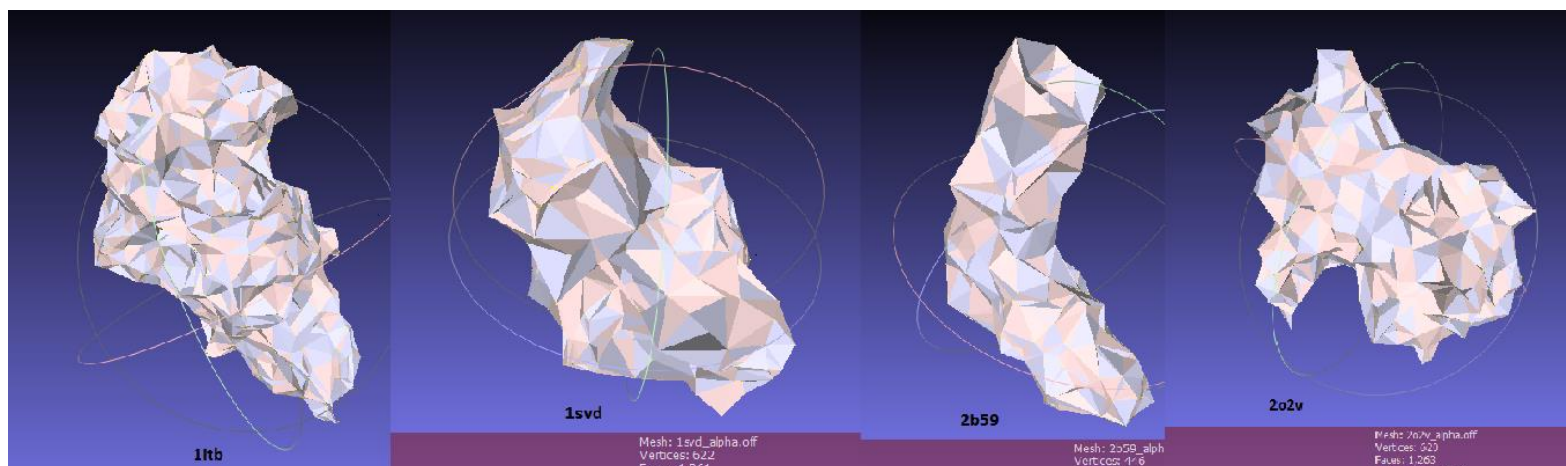
2omz in Chimera



2omz Alpha Shape in MeshLab

Alpha shape of Sample Test Inputs:

- 1itb
- 1svd
- 2b59
- 2o2v



Please find the attached source code