Biogeometry: Molecular Shape Representation Using Delaunay Triangulation

Xinwei Shi
xshi@ucdavis.edu
Genome Center, UC Davis
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A molecule is a collection of at least two atoms held together by chemical bonds.

An atom is a solid objects centered at its nucleus carrying an electrical charge.

Geometrically, we consider each atom as a ball with a specific center and radius; a molecule can be viewed as a union of balls.
Number of atoms in a molecule ranges from 2 to millions.
Geometry is central

Unfolded State

Folded State
Geometry is central

Function depends
On protein shape
Geometric Computing for Studying Biomolecules

- Visualization of proteins and DNAs
- Size and measures
- Shape similarity and complementarity
- Shape deformation
- Simulations
Molecular Shape Representation

- Three existing surface models for molecules

(a) Van der Waals surface
(b) Solvent accessible surface
(c) Molecular surface
Molecular Shape Representation

- Disadvantage
  - Lack of smoothness

An example of the self-intersection of molecular surface
A New paradigm--Skin Surface

- Edelsbrunner, 1998 (part of the alpha shape theory)
- Based on a framework using Delaunay triangulation and Voronoi diagram
- Meshing of skin surfaces using Delaunay triangulation
Skin Definition
Skin surface

- A skin $F_B$ is specified by a set of weighted point $B = \{b_i = (z_i, w_i) \in R^d \times R \mid i = 1, \ldots n\}$
- In three dimensions, the skin surface is a tangent smooth surface free of self-intersection
Sphere Algebra

- **Addition**
  \[(z_i, w_i) + (z_j, w_j) = (z_i + z_j, w_i + w_j + 2 < z_i, z_j >)\]

- **Scalar multiplication**
  \[c \cdot (z_i, w_i) = (c \cdot z_i, c \cdot (w_i - (1 - c) \| z_i \|^2))\]

- **Shrinking**
  \[(z_i, w_i)^{1/2} = (z_i, w_i / 2)\]

\[
\sqrt{B} = \{ \sqrt{b_i} \mid b_i \in B \}
\]

- \(c\) real number; \(<, >\) dot product
Convex Hull of \( B \)

\[
\text{aff} \ (B) = \left\{ \sum_{b_i \in B} \lambda_i b_i \mid \sum_{i} \lambda_i = 1 \right\}
\]

\[
\text{conv} \ (B) = \left\{ \sum_{b_i \in B} \lambda_i b_i \mid \sum_{i} \lambda_i = 1, \forall \lambda_i \geq 0 \right\}
\]
Lifting Map

- Every circle in $\mathbb{R}^2$, its projection under the lifting map is the intersection of the paraboloid with a three dimensional plane.
Lifting Map $\Pi$

$$(x, y) \in \mathbb{R}^2 \Rightarrow (x', y', z) \in \mathbb{R}^3, \quad z = x^2 + y^2$$

$$b_i = (z_i, w_i), \quad z_i = (p, q), \quad r = \sqrt{w_i}$$

$$(x-p)^2 + (y-q)^2 = r^2 = w_i$$

$$x^2 + y^2 = 2px + 2qy - (p^2 + q^2 - w_i)$$

That is, $z = 2px + 2qy - (p^2 + q^2 - w_i)$

plane with normal $\frac{\tilde{b}_i}{\sqrt{2}}$ $2p, 2q, -1$

Remark 1: $(xy)$ in the circle, $x^2 + y^2 < w_i$, above the plane on the intersection outside under the plane

$R: 2$

$w_i > 0, \quad P \cap \Pi \neq \emptyset$

$w_i = 0, \quad P \cap \Pi = \mathbb{R}$

$w_i < 0, \quad$ under $\Pi$, imaginary circle

Voronoi paper 1907/08
Del paper 1930.
Lifting Map

- Convex hull of a set of circles is the projection of the upper hull of their lifting planes
Convex combination

\[ \forall b_j \in \text{aff}(B) \]

\[ z_j = \sum_i \lambda_i z_i, \]

\[ w_j = \sum_i \lambda_i w_i + \left\| \sum_i \lambda_i z_i \right\|^2 - \sum_i \lambda_i \|z_i\|^2. \]
2. Proof by deduction
   Center and Radius of \( \lambda_0 \mathbf{b}_0 + \lambda_1 \mathbf{b}_1 \)
   \[
   \mathbf{b}_0 = (z_0, w_0) \quad \mathbf{b}_1 = (z_1, w_1)
   \]
   \[
   \lambda_0 \mathbf{b}_0 = (\lambda_0 z_0, \lambda_0 (w_0 - (1 - \lambda_0) ||z_0||^2))
   \]
   \[
   \lambda_1 \mathbf{b}_1 = (\lambda_1 z_1, \lambda_1 (w_1 - (1 - \lambda_1) ||z_1||^2))
   \]
   \[
   \lambda_0 \mathbf{b}_0 + \lambda_1 \mathbf{b}_1 = (\lambda_0 z_0 + \lambda_1 z_1, \frac{2 \lambda_0 z_0 \cdot \lambda_1 z_1 + \lambda_0 ||z_0||^2 + \lambda_1 ||z_1||^2}{||\lambda_0 z_0 + \lambda_1 z_1||^2}
   \]
   \[
   + \frac{\lambda_0 w_0 + \lambda_1 w_1, \Sigma \lambda_i w_i}{||\lambda_0 z_0 + \lambda_1 z_1||^2}
   \]
   \[
   - \lambda_0 ||z_0||^2 - \lambda_1 ||z_1||^2
   \]
   \[
   - \frac{\Sigma \lambda_i ||z_i||^2}{||\lambda_0 z_0 + \lambda_1 z_1||^2}
   \]

3. Orthogonal sphere
   \[
   \mathbf{b}_i \perp \mathbf{b}_j \quad \text{iff} \quad \Pi (\mathbf{b}_i, \mathbf{b}_j) = ||z_i - z_j||^2 - w_i - w_j = 0
   \]
An example when $\text{card}(B) = 2$ in $\mathbb{R}^2$
Orthoanality

- Two circles are called orthogonal circles if only if their weighted distance is zero
Revisit Lifting Map

- Each point on the lifting plane is corresponding to a orthogonal circle of its preimage
4. Map a point in 3D to a circle

\[(m, n, t) \mapsto b_j = (z_j, w_j)\]

\[z_j = (m, n), \quad w_j = m^2 + n^2 - t\]

\[\Pi(b_i, b_j) = \Pi(z_i - z_j) - w_i - w_j = (p - m)^2 + (q - n)^2 - w_i - (m^2 + n^2 - t)\]

\[= (2pm + 2qn - (p^2 + q^2 - w_i) + t\]

\[= 0\]

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5. If \( b_i \perp b_j \), \( b_i \perp b_j \Rightarrow b_k \perp b \in \operatorname{Alt}(b_i, b_j) \)

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6. If \( b_i \perp b_j \), \( \sqrt{b_i} \cap \sqrt{b_j} = \bigcup_{x} \{ w_i = w_j \} \)

Proof: \( \sqrt{b_i} = (z_i, \frac{w_i}{2}) \)

\[\sqrt{b_j} = (z_j, \frac{w_j}{2})\]

\[\Pi(z_i - z_j)^2 = w_i + w_j\]

\[\Rightarrow w_i + w_j - \left(\frac{\sqrt{2w_i}}{2} - \frac{\sqrt{2w_j}}{2}\right)^2\]

\[= \left(\frac{\sqrt{2w_i}}{2} + \frac{\sqrt{2w_j}}{2}\right)^2\]
Coaxal system
Shrinking
An **envelope** of a family of curves in the plane is a curve that is tangent to each member of the family at some point.
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Envelope

\[(x-2)^2 + y^2 = z^2 + 1\]

After shrinking

\[f(2, x, y) = (x-2)^2 + y^2 - \frac{(z^2+1)}{2}\]

\[\frac{\partial f}{\partial z} = -2(x-2) - 2z = 2 - 2x = 0\]

\[z = 2x\]

\[f(2x, x, y) = x^2 + y^2 - \frac{4x^2+1}{2}\]

\[= -x^2 + y^2 - \frac{1}{2}\]
Skin and body

- For a general finite set $B$, the skin $F_B$ is the envelope of the shrinking convex hull of $B$:

$$SKN_B = \text{env}(\sqrt{\text{conv}(B)})$$

$$BDY_B = \bigcup(\sqrt{\text{conv}(B)})$$
The Example

- $B = \{b_1, b_2\}$

$\text{conv}(B)$

$\sqrt{\text{conv}(B)}$

$\text{env}(\sqrt{\text{conv}(B)})$
Another Example
Complementarity

- The orthogonal sphere set of $B$, $B^\perp$, specifies the same skin as $B$

\[
\text{body}(B) \bigcap \text{body}(B^\perp) = \text{skin}(B) = \text{skin}(B^\perp),
\]

\[
\text{body}(B) \bigcup \text{body}(B^\perp) = \mathbb{R}^3.
\]
An example

The molecular skin model of protein gramcidA. and a complementary portion
Skin Decomposition
• A skin is composed of a set of quadratic pieces that joined each other smoothly
• We can decompose a skin surface into simple pieces using the Delaunay triangulation and its dual Voronoi diagram
Weighted Delaunay Triangulation

Weighted Voronoi Diagram and Delaunay triangulation defined by 4 spheres in $\mathbb{R}^2$
Mixed Complex

- The *mixed complex* $M_B$ partition the space to convex polyhedra

Mixed complex:

shrinking Minkowski sum

$$M_B = (D_B \oplus V_B) / 2 = \bigcup_{X \subset B} \mu_X$$

Weighted Delaunay triangulation $D_B$

Weighted Voronoi Diagram $V_B$
Skin decomposition

- The skin clipped in each mixed cell is quadratic

\[ F_B \cap \mu_X = \text{env}(\sqrt{\text{aff}(X)}) \cap \mu_X \]

In 2 dimensions,
- \( \text{card}(X) = 1 \), sphere
- \( \text{card}(X) = 2 \), hyperbola
- \( \text{card}(X) = 3 \), sphere (inverse)
Mixed Cells in $\mathbb{R}^3$
Quadratic Patches in $\mathbb{R}^3$
Complexity

- Number of quadratic patches in the skin surface specified by $n$ spheres can $O(n^2)$
- For molecules, the number of patches is usually linear to the number of atoms
Three dimensional example

Sphere patches

Hyperboloid patches

card(X) = 1, 4

card(X) = 2, 3
Skin surfaces

A protein

Face model
Skin surfaces
Adaptive Meshing
Meshing

- A meshing, or triangulation of a surface $F$ is a simplicial complex whose underlying space is homomorphic to $F$.
- Geometry preserved
  - Hausdorff distance between the surface and mesh has a upper bound
- High mesh quality.
  - The smallest angle of the mesh has a lower bound
Simplicial Complex

- Simplex

- Simplicial complex and its underlying space
Homeomorphism

- A map $f$ is a homeomorphism if it is bijective and has a continuous inverse.
Adaptive

- Triangle size in the adapts the local surface geometry
Curvature -- Plane curves

\[ \kappa(x) = \|\ddot{\gamma}(x)\| = \frac{1}{r} \]
Surface curvature

- Principle Normal Curvature

- Euler’s formula (1760)
Curvature of skin surface

- Constant curvature \((1/R)\) on spherical patches
- On a hyperboloid, the maximum more curvature is 1 over the radius of sandwiching sphere
Curvature variation

- The radius of the maximum curvature \((local \ length \ scale)\) of the skin surface satisfies the 1-Lipschitz condition,

\[
|\rho(x) - \rho(y)| \leq \|x - y\|.
\]

- This property implies that the curvature varies slowly on the surface.
The local length scale at a point $x$ on the skin surface is the lower bound of the local feature size $lfz(x)$.
Adaptive Meshing

- Generation of an adaptive sampling.
- Construct a triangulation using the samples.
\( \varepsilon \)-sampling of the Skin Surface

- A dense sample points set in terms of the local length scale

\( r = \varepsilon \rho(x) \)
Restricted Delaunay triangulation

• A set of points $T \subseteq F_B$
• Restricted Voronoi polygon of $a \in T$
  \[ \nu'_a = \nu_a \cap F_B \]
• Restricted Voronoi Diagram $V_T = \bigcup \nu'_a$, $a \in T$, $\nu'_a \neq \emptyset$
• Restricted Delaunay triangulation $D_T'$ of $F_B$
  is the dual of $V_T$
Homeomorphism Theorem

- Closed Ball Property
ε need to be small

- Require ε < 0.179 for skin surfaces
- Precise approximation of the geometry as well
Even $\varepsilon$-sampling

- Two sample points should not be too close to each other

$$r = \varepsilon \varrho(x)$$

$$r = \gamma \varrho(t), t \in T$$
Skin Meshing using Restricted Union of Balls
Overview of the algorithm

- Generate an even $\varepsilon$-sampling incrementally
- Construct the Delaunay triangulation of the sample points simultaneously
- Extract the restricted Delaunay triangulation as the surface mesh
Even $\varepsilon$-sampling

- Using a set of $r$ balls,
- Restricted union of balls: the intersection of the union of $r$ balls and the skin surface

$$r = \gamma g(t), t \in T$$
Observation

- If the restricted union of balls covers the whole surface with some feasible $r$ value, the RDT of the sample points is homeomorphic to the surface and has a lower bound on its minimum angle.
Theorem

- If the restricted union of balls covers the whole surface with $0 < r < \varepsilon/(1 + \varepsilon)$, the RDT of the sample points is homeomorphic to the surface and has a lower bound $20^\circ$ on its minimum angle.
Construct the Restricted Union of Ball

- Start from four seed point,
- Add new points and put $r$ balls on the boundary of the RUB
- Compute the Delaunay triangulation and extract surface triangles and update the front
Extract surface triangles

- **Small radius property**
  \[ R_{abc} < \frac{\varepsilon}{1 - \varepsilon} \rho_{abc}. \]

- **Restricted Delaunay property**
  \[ \|oz\| \leq \frac{\varepsilon^2}{2} \rho_{abc}, \]
  \[ \rho_{abc} = \min\{\rho(a), \rho(b), \rho(c)\} \]
Surface Mesh
More examples
Mesh Quality

Skin model for a protein
## Quality statistics

<table>
<thead>
<tr>
<th>molecular name</th>
<th>no. triangles in the mesh</th>
<th>minimum angle distribution(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>50°-60°</td>
</tr>
<tr>
<td>Helix</td>
<td>98,017</td>
<td>58.21</td>
</tr>
<tr>
<td>HIV2</td>
<td>226,758</td>
<td>56.22</td>
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<td>1CHO</td>
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<td>56.00</td>
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<tr>
<td>1ACB</td>
<td>290,476</td>
<td>56.20</td>
</tr>
</tbody>
</table>

Table 4.2: Triangle quality distribution.
Tetrahedral Meshes
Initial Tetrahedralization

- Build a coarse tetrahedral mesh for the volume from the surface mesh
Tetrahedral Quality

- Radius-edge ratio

**Skinny tetrahedra** \( \frac{r}{l} \geq C \)
**Quality Improvement**

- **Delaunay Refinement**
  - Insert the circumcenter of the skinny tetrahedron iteratively
Challenges

• **Boundary protection**
  • The circumcenter of a skinny tetrahedron may be outside the skin volume
  • Result of the tetrahedral mesh not conform to the boundary
Prioritized Delaunay Refinement

- Insert the circumcenters from the region inside the skin volume to the region near the surface, so that,
- The circumcenters of the skinny tetrahedra are always inside the volume.
Prioritized Delaunay Refinement

- **Distance function**

\[ d(x) = \inf_{p \in F_B} \|x - p\|, \forall x \in \mathbb{R}^3. \]
Prioritized Delaunay Refinement
An examples
Results
Calculating Molecular Electrostatics

- **Poisson Boltzmann equation** describes the electrostatic potential using the continuum model of molecules in ionic solution

\[
\nabla^2 \phi_1(x) = \sum_{i=1}^{N_m} \frac{-4\pi q_i}{\epsilon_1} \delta(x - x_i)
\]

\[
\nabla^2 \phi_2(x) = \kappa^2 \frac{k_BT}{e_c} \sinh\left(\frac{e_c \phi_2(x)}{k_BT}\right)
\]

\[
- \nabla \cdot (\epsilon(x) \nabla \phi(x)) + \kappa^2(x) \sinh\left(\frac{e_c \phi(x)}{k_BT}\right) = 4\pi \sum_{i=1}^{N_m} q_i \delta(x - x_i)
\]
Multigrids Method for Solving PBE

- Construct of a hierarchy of meshes
- Solve the system at the coarsest mesh
- Get the solution of the fine mesh step by step using coarse meshes
Mesh Coarsening
Hierarchical Mesh
Mesh Coarsening

- **Constraints:**
  - Mesh quality, Topology Correctness, Approximation Accuracy, Adaptive to the Curvature, and Restricted Delaunay Property.
Adaptive Mesh

\[ [L_i] \quad R_{ab} > \frac{C_i}{Q_i} \rho_{ab}, \text{ for every edge } ab, \]
\[ [U_i] \quad R_{abc} < C_i Q_i \rho_{abc}, \text{ for every triangle } abc. \]


**Algorithm 1 CoarsenSkinMesh**($C_i, Q_i, F_B, T_{i-1}$)

1: while eq is not empty do
2:    $ab = \text{deQueue}(eq);$ 
3:    edgeContraction($ab$); 
4:    Update $fs$; 
5:    flipEdges($fs$); 
6:    Update $eq$ and $ts$; 
7:    vertInsertion($ts$); 
8:    Update $fs$; 
9:    flipEdges($fs$); 
10: end while
Results
Fig. 8. A comparison of our skin mesh coarsening algorithm with Qslim.
Discussions

• Render skin surfaces using ray tracing
• New idea for meshing
• Medial Axis of Skin
• Modeling other objects other than molecule
• Deformation
Questions