Biogeometry: Molecular Shape Representation Using Delaunay Triangulation

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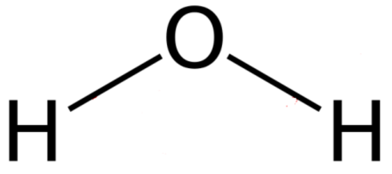
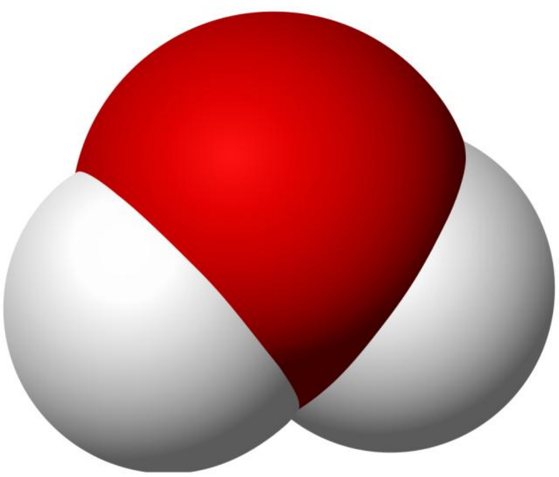
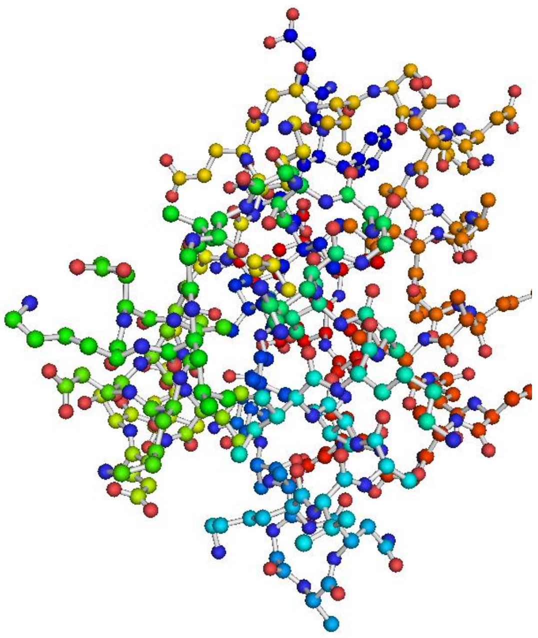
Molecule

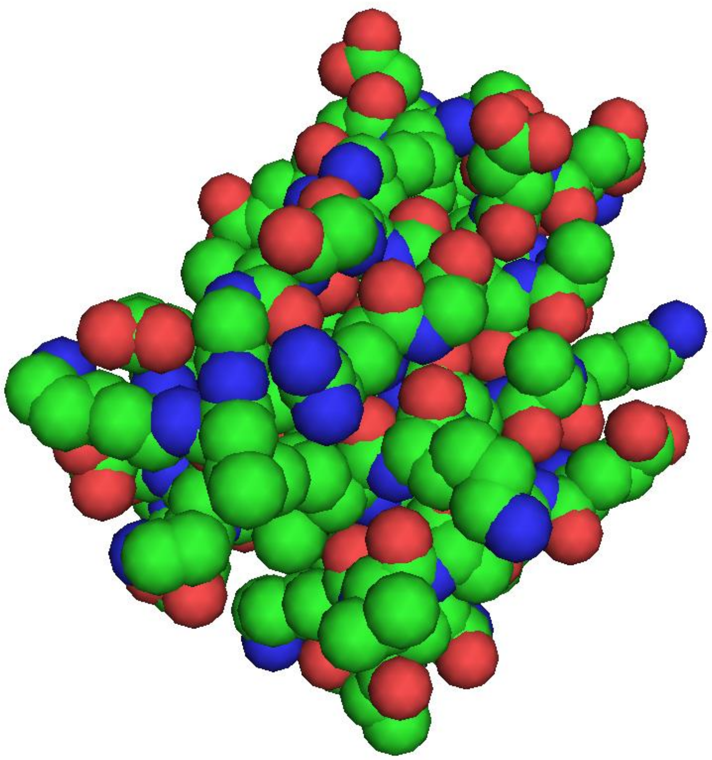
- A **molecule** is a collection of at least two **atoms** held together by chemical bonds
- An **atom** is a solid objects centered at its nucleus carrying an electrical charge
- Geometrically, we consider each atom as a ball with a specific center and radius; a molecule can be viewed as a union of balls.

Molecule



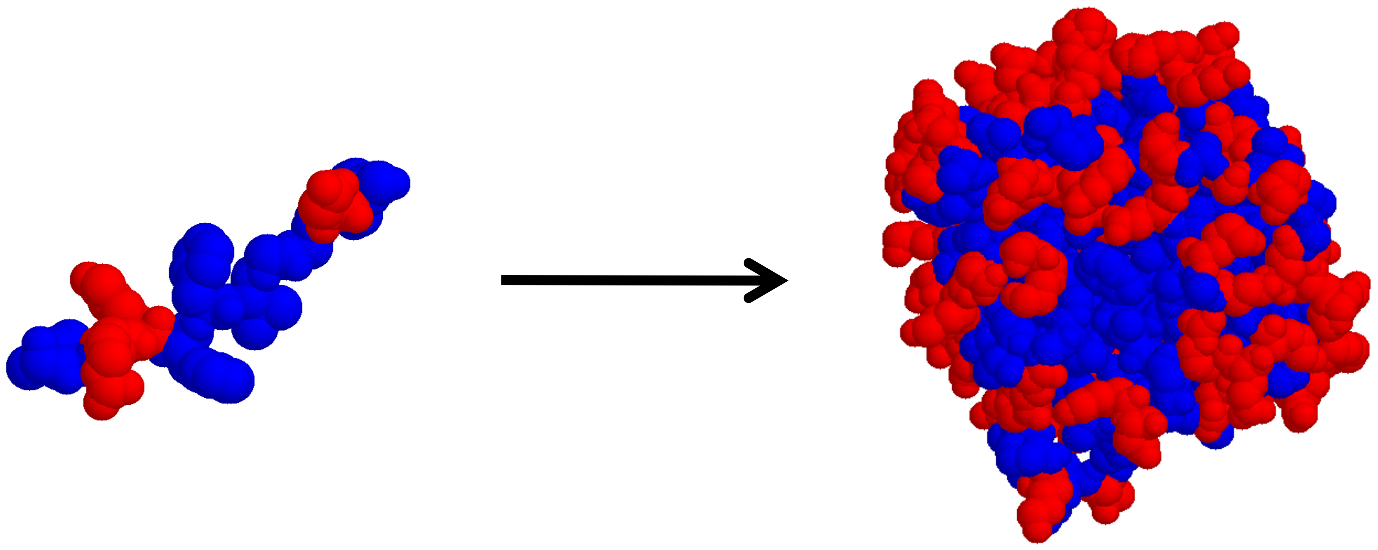






Number of atoms in a molecule ranges from 2 to millions

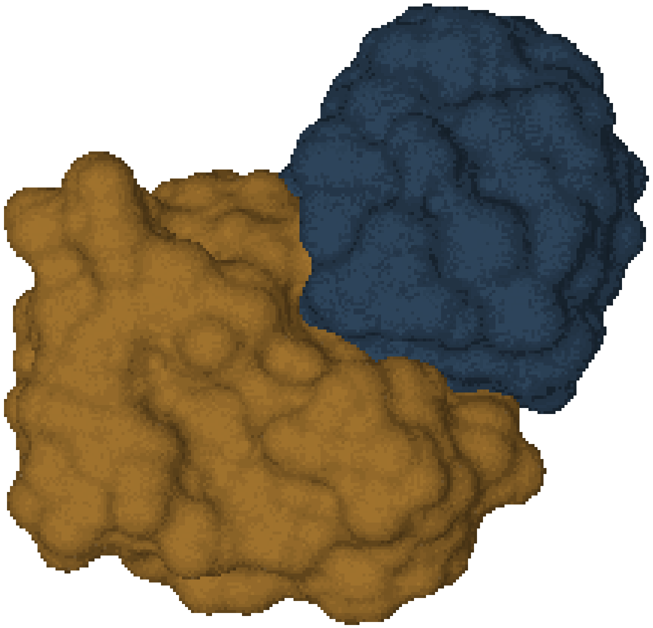
Geometry is central

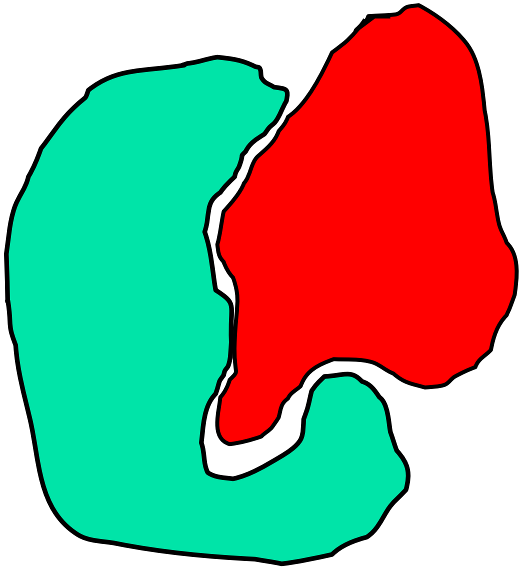


Unfolded State

Folded State

Geometry is central





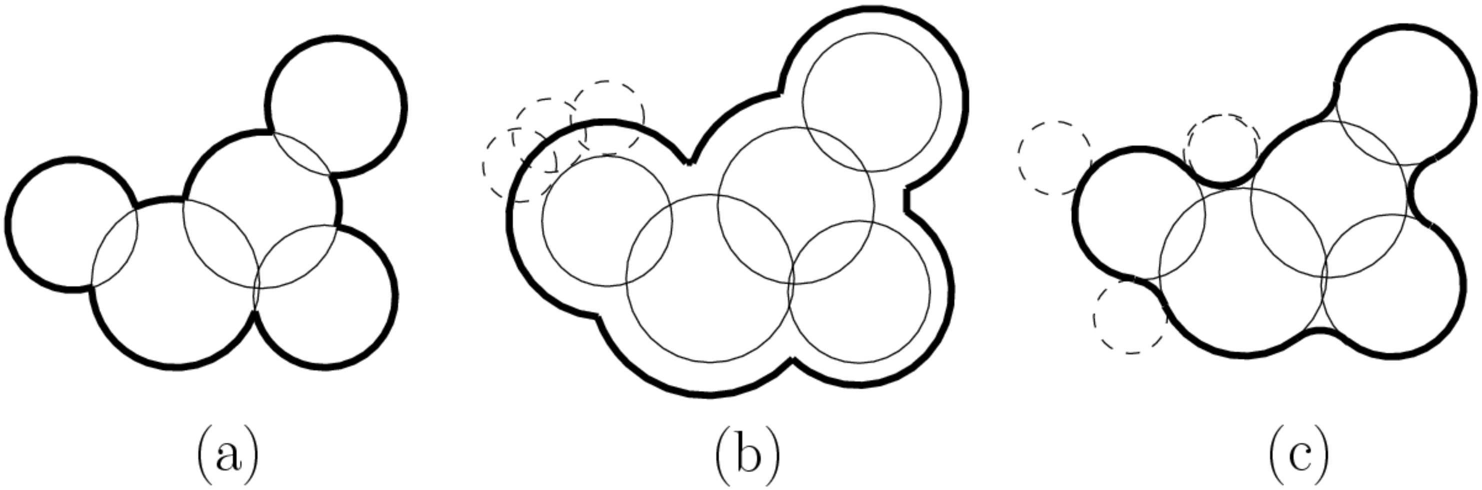
Function depends
On protein shape

Geometric Computing for Studying Biomolecules

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

Molecular Shape Representation

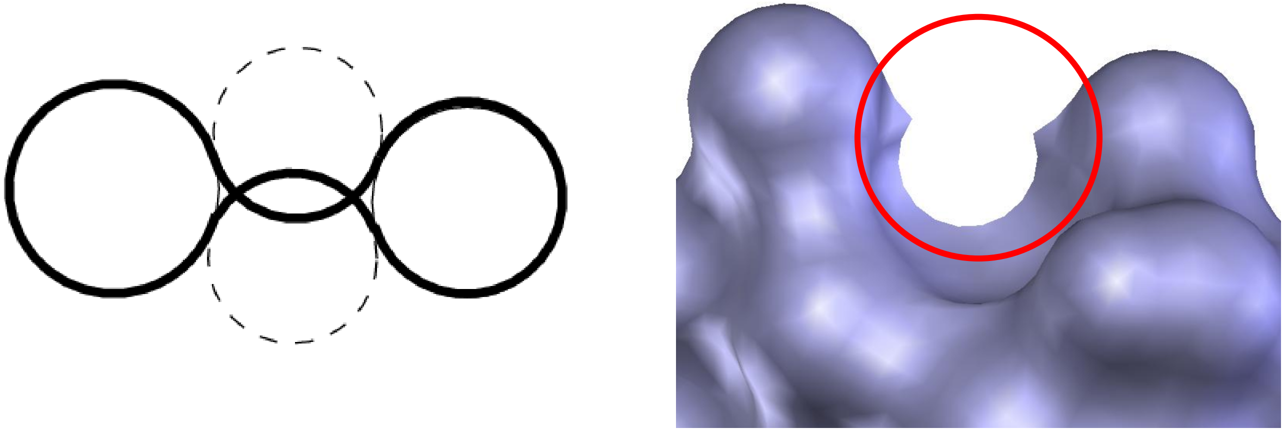
- Three existing surface models for molecules



Van der Waals surface   Solvent accessible surface   Molecular surface

Molecular Shape Representation

- Disadvantage
  - Lack of smoothness



An example of the self-intersection of molecular surface

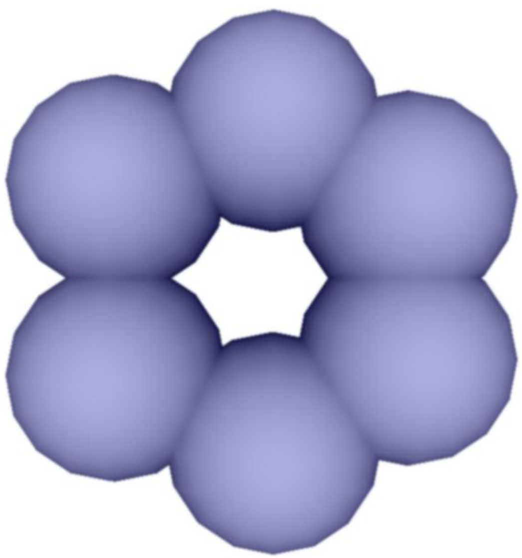
A New paradigm--Skin Surface

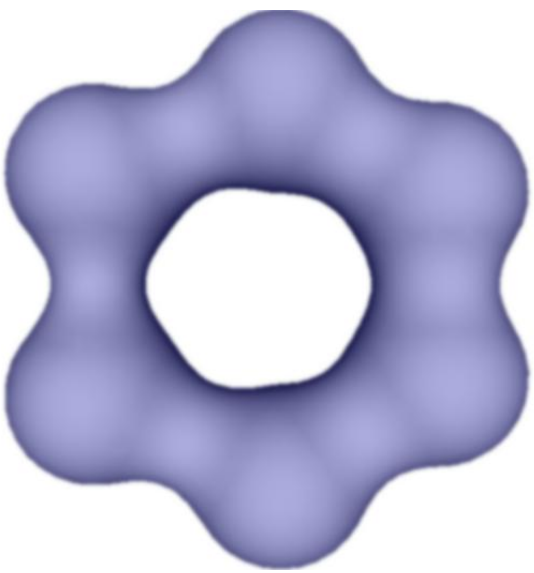
- Edelsbrunner, 1998 (part of the alpha shape theory)
- Based on a framework using Delaunay triangulation and Voronoi diagram
- Meshing of skin surfaces using Delaunay triangulation

Skin Definition

Skin surface

- A skin F_B is specified by a set of weighted point $B = \{b_i = (z_i, w_i) \in R^d \times R \mid i = 1, \cdots n\}$
- 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

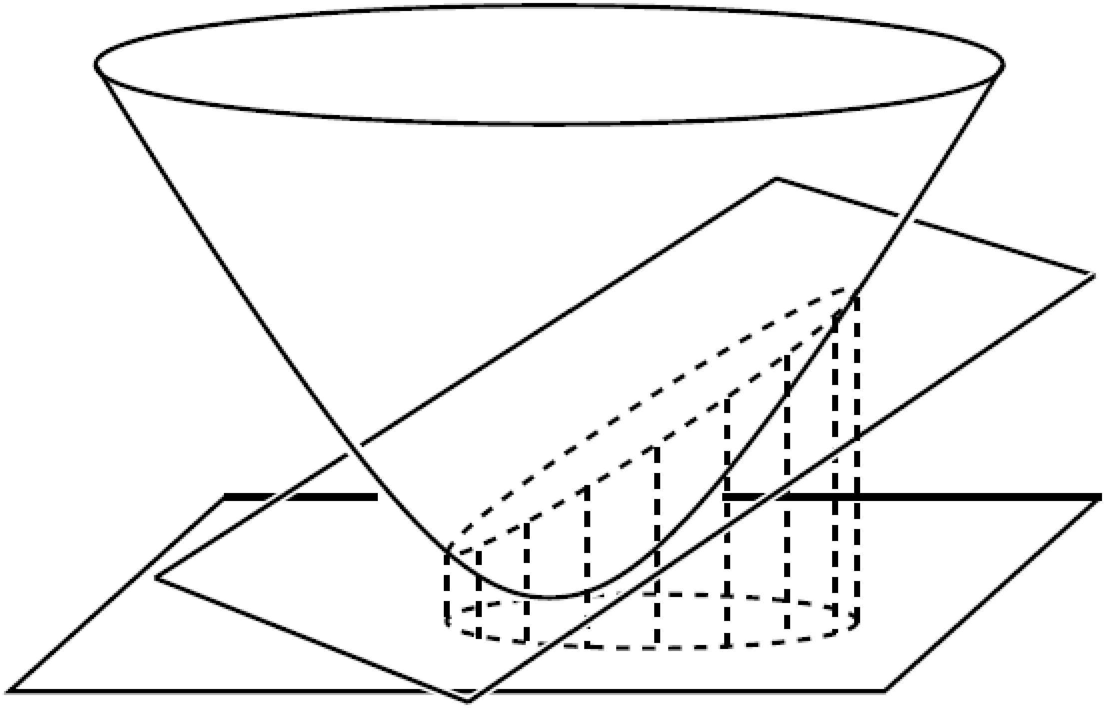
Convex Hull of B

$$\operatorname{aff}(B) = \{ \sum_{b_i \in B} \lambda_i b_i \mid \sum_i \lambda_i = 1 \}$$

$$\operatorname{conv}(B) = \{ \sum_{b_i \in B} \lambda_i b_i \mid \sum_i \lambda_i = 1, \forall \lambda_i \geq 0 \}$$

Lifting Map

- Every circle in R^2, its projection under the lifting map is the intersection of the paraboloid with a three dimensional plane



slides 14:

1) Lifting Map Π

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

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

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

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

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

plane with normal P_i $(2p, 2q, -1)$

Remark 1: (x,y) in the circle, $x^2+y^2 < w_i$, above the pl

on : intersetion

outside under the plane

R.2 $w_i > 0$, $P_n \cap \Pi \neq \phi$

$w_i = 0$ $P \cap \Pi = x$

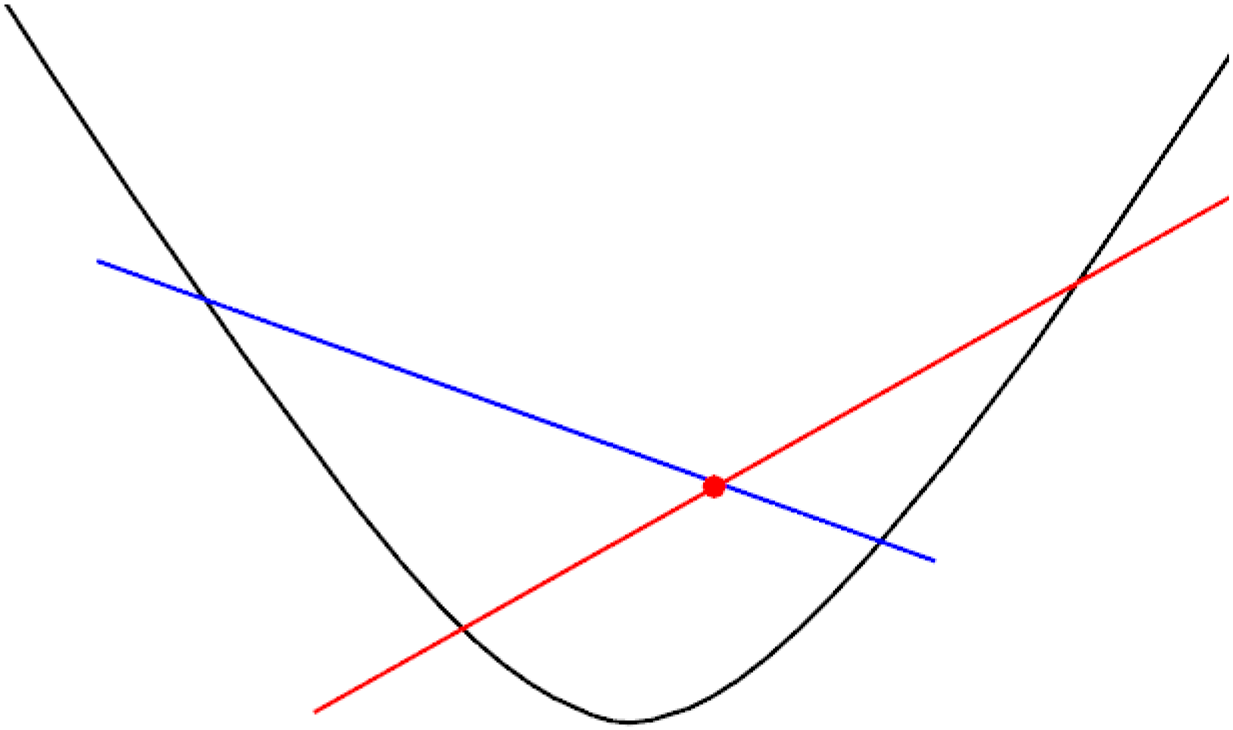
$w_i < 0$ under Π, imaginary circle

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

$$\forall b_j \in \text{aff}\,(B)$$

$$\begin{aligned} z_j &= \sum_i \lambda_i z_i, \\ w_j &= \sum_i \lambda_i w_i + \left\| \sum_i \lambda_i z_i \right\|^2 - \sum_i \lambda_i \| z_i \|^2. \end{aligned}$$

Slides 16: ②

2. proof by deduction

Center and Radius of $\lambda_0 b_0 + \lambda_1 b_1$

$$b_0 = (z_0, w_0) \quad b_1 = (z_1, w_1)$$

$$\lambda_0 b_0 = (\lambda_0 z_0,\ \lambda_0 (w_0 - (1-\lambda_0)\|z_0\|^2))$$

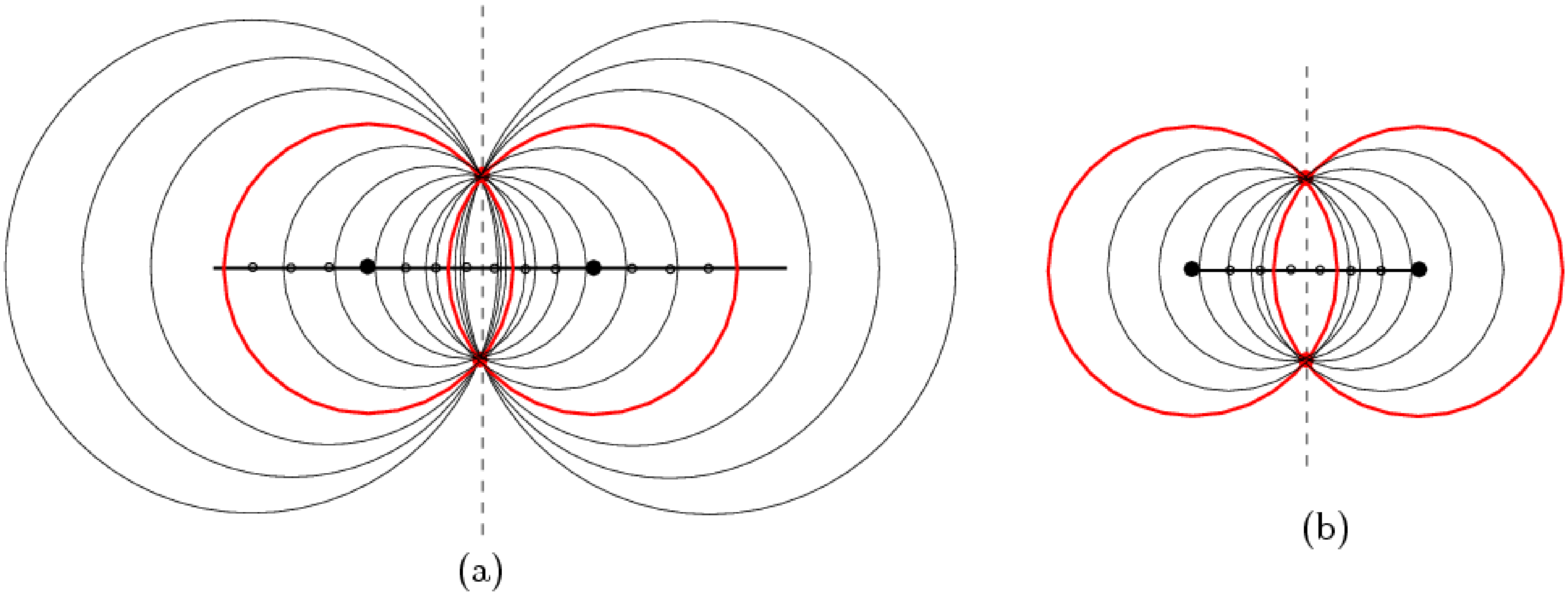
$$\lambda_1 b_1 = (\lambda_1 z_1,\ \lambda_1 (w_1 - (1-\lambda_1)\|z_1\|^2))$$

$$\lambda_0 b_0 + \lambda_1 b_1 = \Big(\underline{\lambda_0 z_0 + \lambda_1 z_1},\ \underbrace{2\langle \lambda_0 z_0, \lambda_1 z_1\rangle + \lambda_0^2\|z_0\|^2 + \lambda_1^2\|z_1\|^2}_{\|\Sigma \lambda_i z_i\|^2} \underbrace{+ \lambda_0 w_0 + \lambda_1 w_1}_{\Sigma \lambda_i w_i} \underbrace{- \lambda_0\|z_0\|^2 - \lambda_1\|z_1\|^2}_{-\Sigma \lambda_i \|z_i\|^2}\Big)$$

3. orthogonal sphere

$b_i \perp b_j$ iff $\Pi(b_i, b_j) = \|z_i - z_j\|^2 - w_i - w_j = 0$

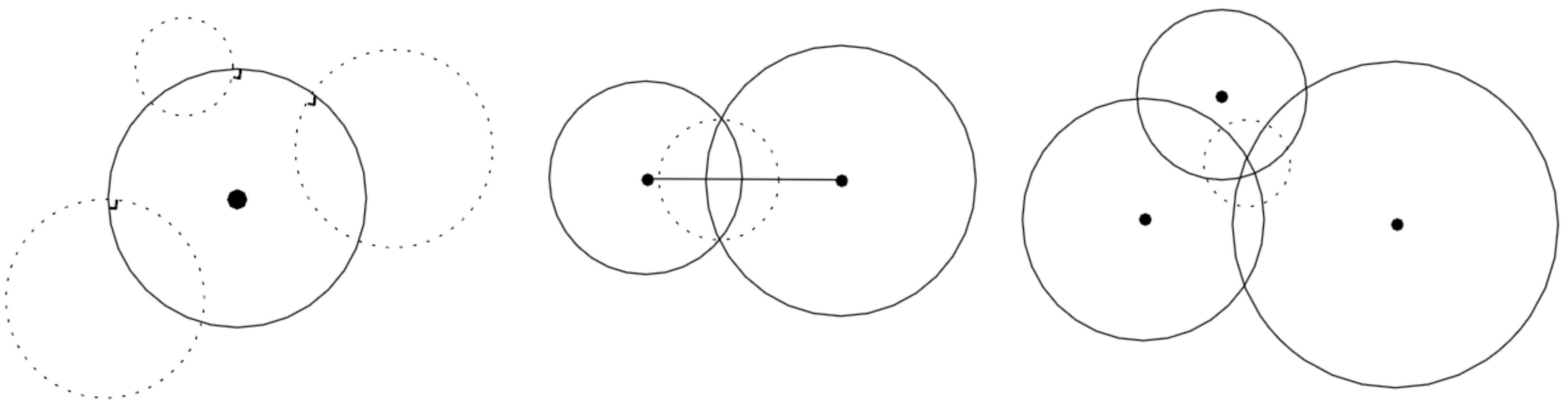
An example



An example when card(B) =2 in R^2

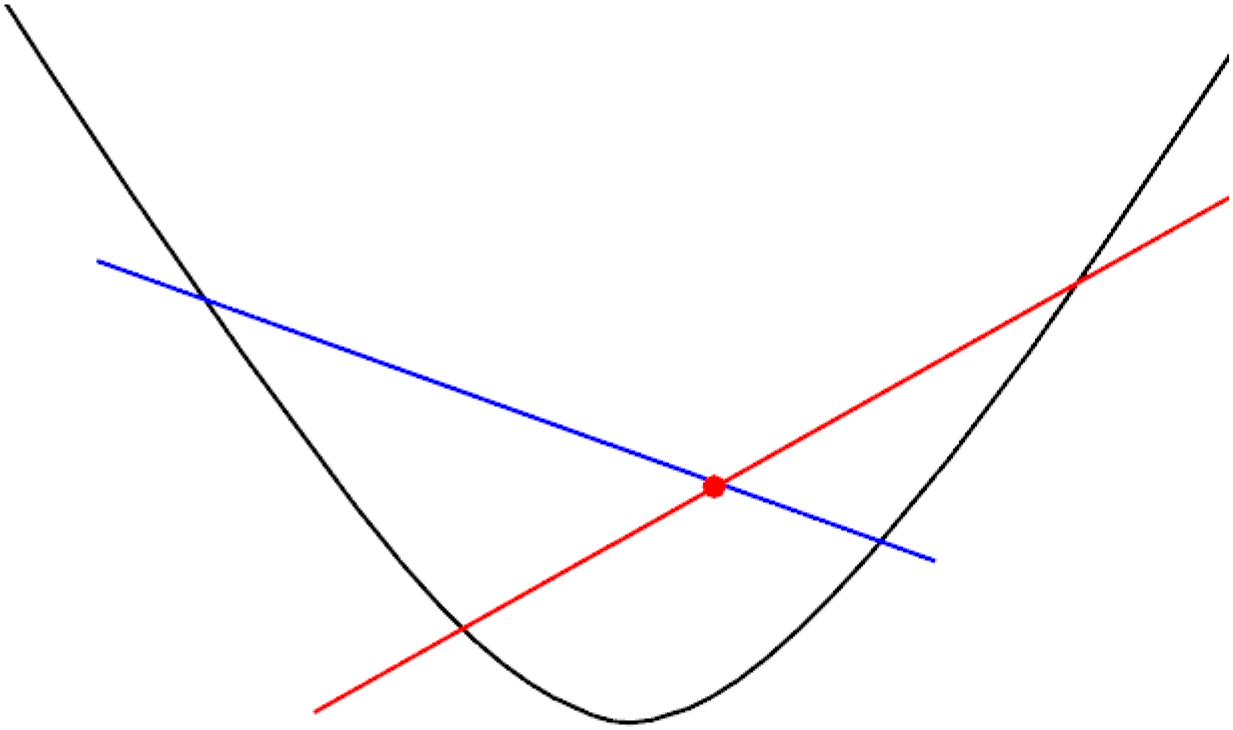
Orthogoanality

- 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



Slides 19 ③

4. Map a point in 3D to a circle

$(m, n, t) \in P_i \Rightarrow b_j = (z_j \ \ w_j)$

$z_j = (m, n) \qquad w_j = m^2 + n^2 - t$

$\Pi(b_i, b_j) = \| z_i - z_j) - w_i - w_j$

$= (p-m)^2 + (q-n)^2 - w_i - (m^2 + n^2 - t)$

$= -(2pm + 2qn - (p^2 + q^2 - w_i) + t$

$= 0$

Slides 20

5. If $b_k \perp b_i$, $b_k \perp b_j \Rightarrow b_k \perp b \in Aff(b_i, b_j)$

Slides 21

6. If $b_i \perp b_j$, $\sqrt{b_i} \cap \sqrt{b_j} = \begin{cases} x & w_i = w_j \\ \phi & \end{cases}$

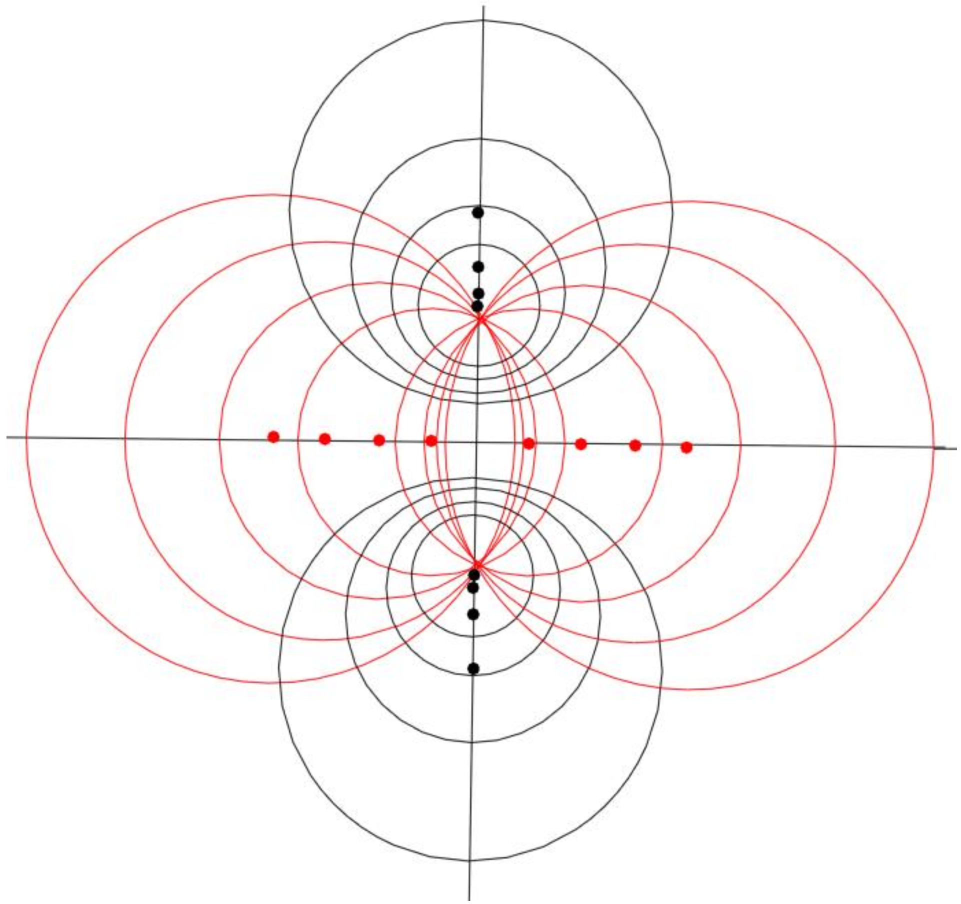
Proof: $\sqrt{b_i} = (z_i, \frac{w_i}{2})$, $\sqrt{b_j} = (z_j, \frac{w_j}{2})$

$\| z_i - z_j \|^2 = w_i + w_j$

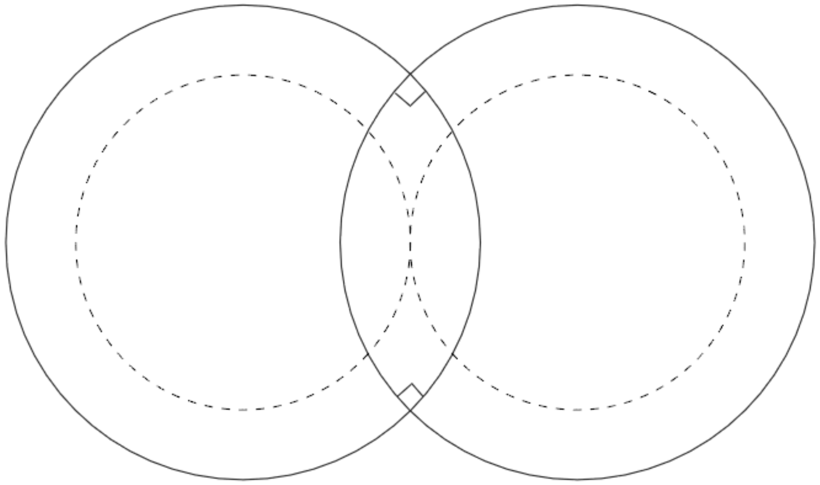
$\geq w_i + w_j - \left(\frac{\sqrt{2w_i}}{2} - \frac{\sqrt{2w_j}}{2}\right)^2$

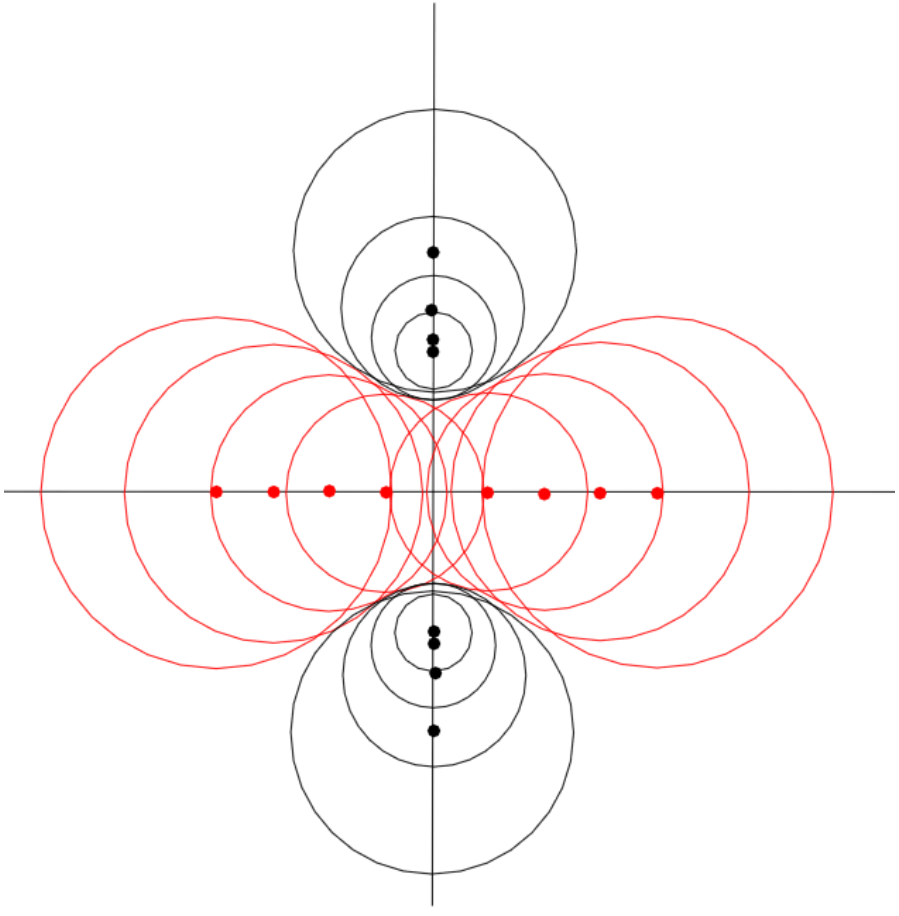
$= \left(\frac{\sqrt{2w_i}}{2} + \frac{\sqrt{2w_j}}{2}\right)^2$

Coaxal system



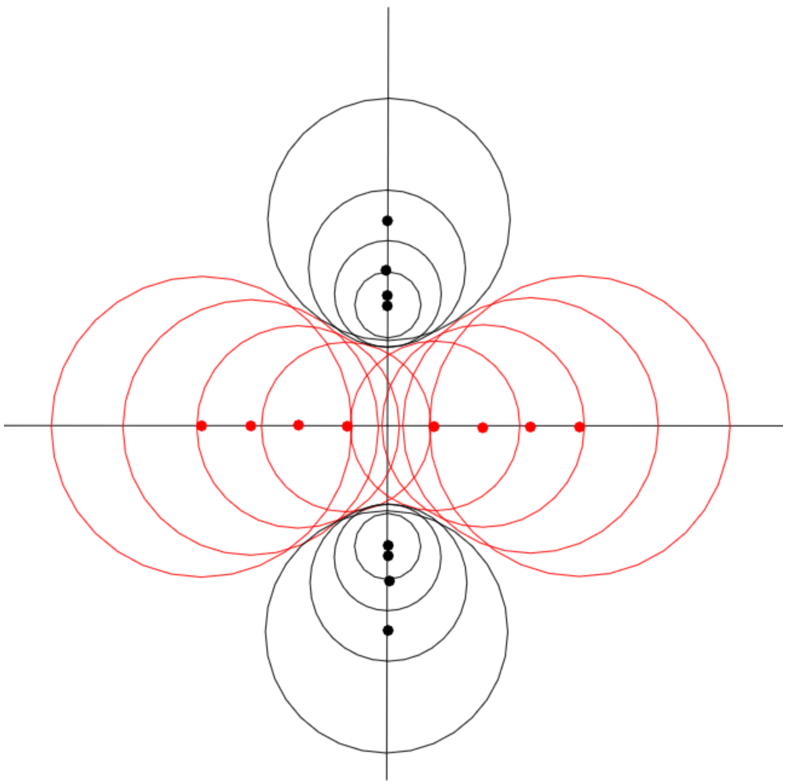
Shrinking

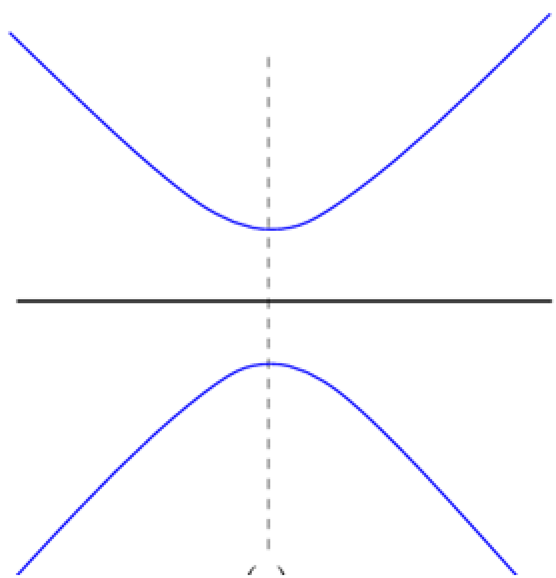




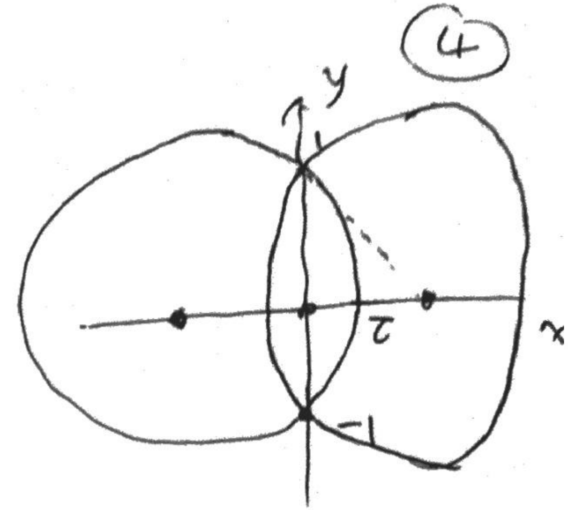
Envelopes

- 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.





7. slides 22



Envelop

$$(x-\tau)^2+y^2=\tau^2+1$$

After shrinking

$$f(\tau, x, y) = (x-\tau)^2+y^2-\frac{(\tau^2+1)}{2}$$

$$\frac{\partial f}{\partial \tau} = -2(x-\tau) - \tau = \tau - 2x = 0$$

$$\tau = 2x$$

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

$$= -x^2+y^2-\frac{1}{2}$$

Skin and body

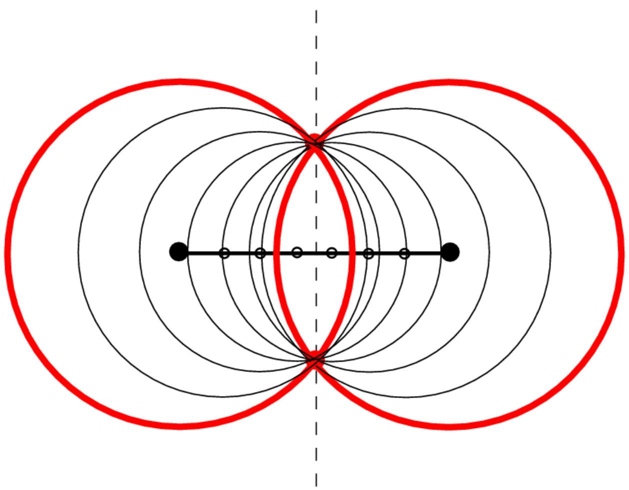
- For a general finite set B, the skin F_B is the envelope of the shrinking convex hull of B:

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

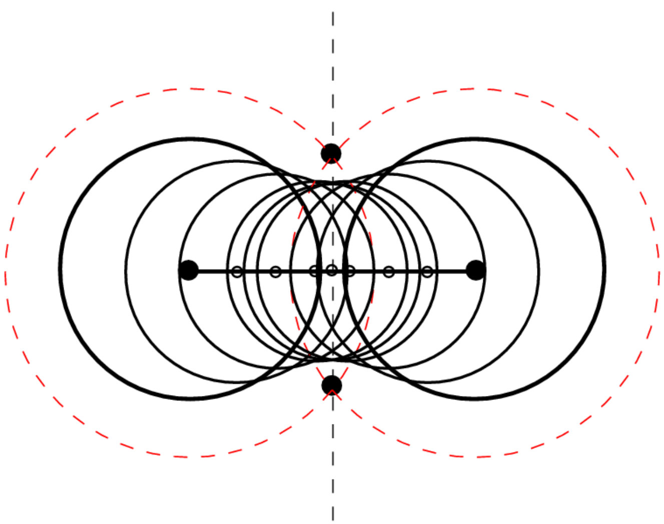
$$BDY_B = \bigcup(\sqrt{conv(B)})$$

The Example

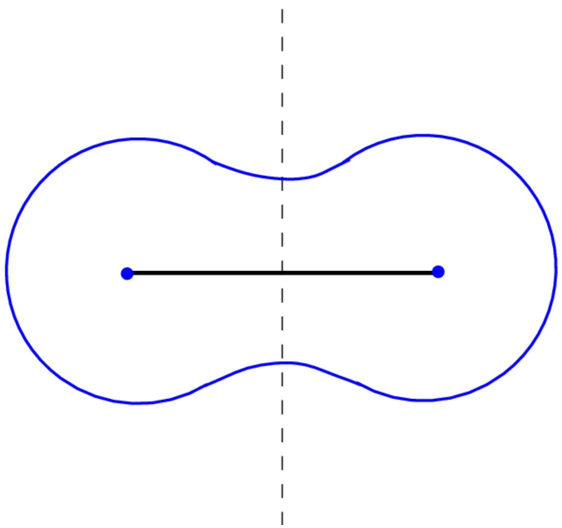
- $B = \{b_1, b_2\}$



$conv(B)$

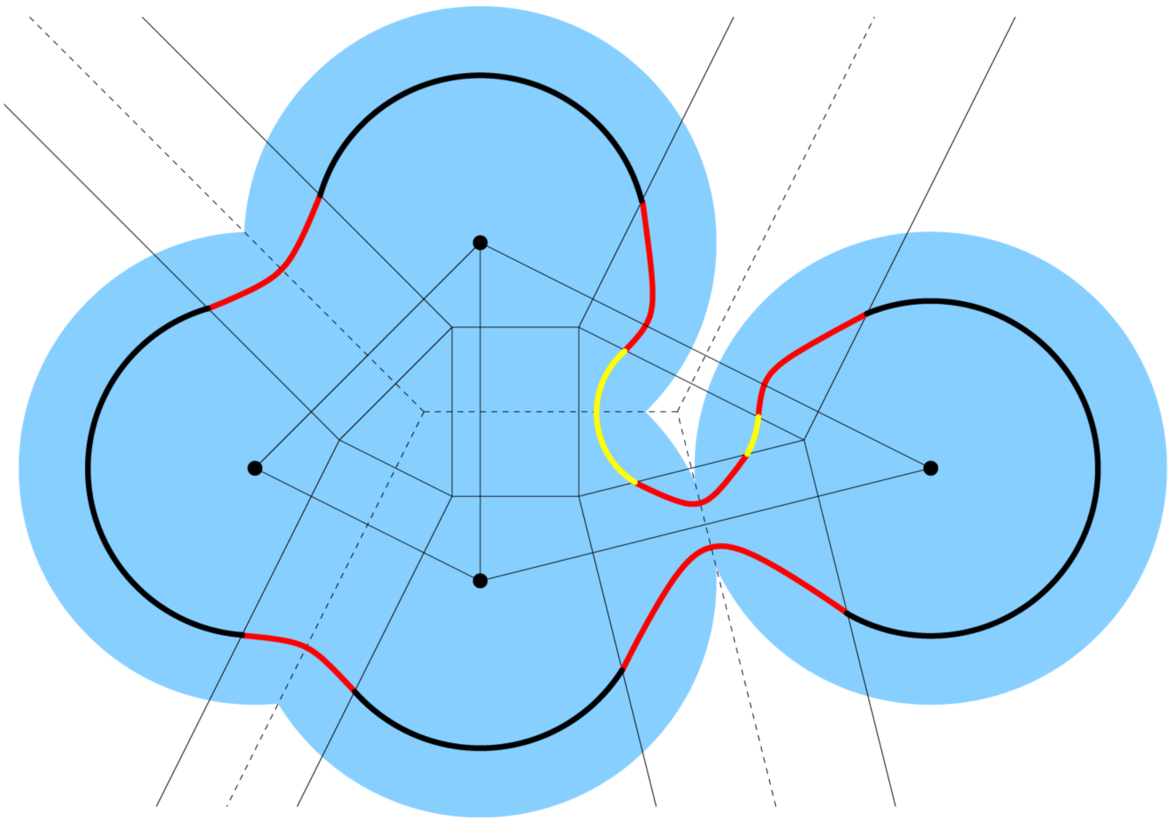


$\sqrt{conv(B)}$



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

Another Example

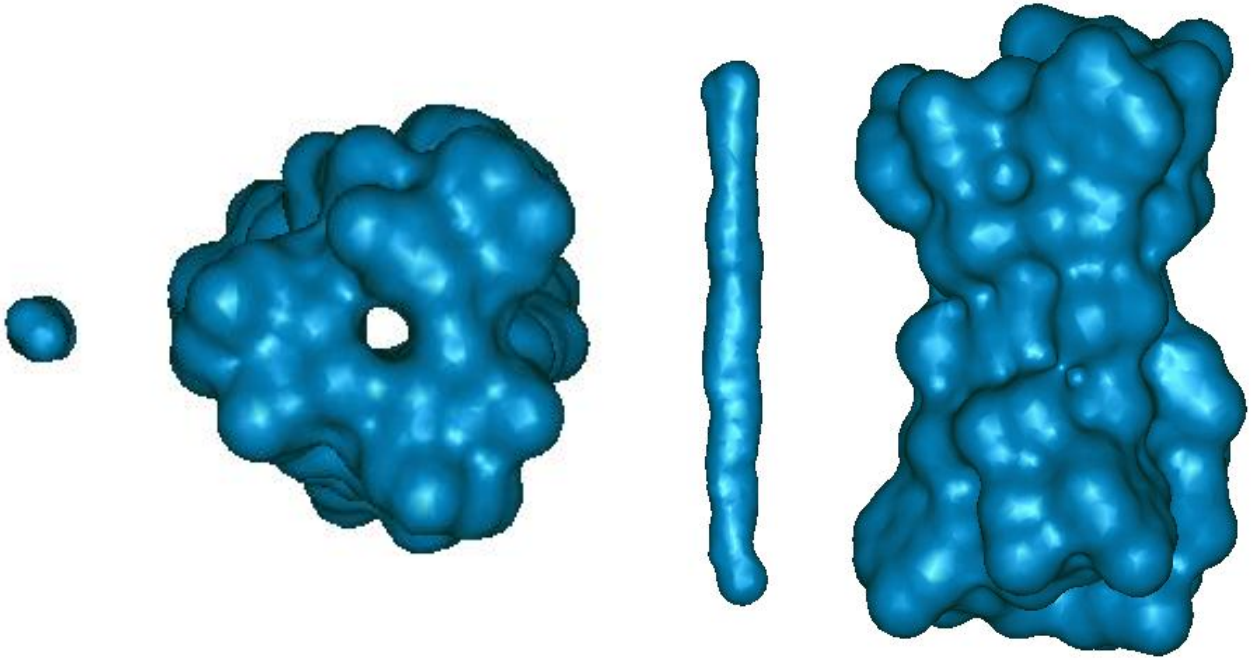


Complementarity

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

$$
\begin{aligned}
\mathrm{body}(B) \bigcap \mathrm{body}(B^{\perp}) &= \mathrm{skin}(B) \\
&= \mathrm{skin}(B^{\perp}), \\
\mathrm{body}(B) \bigcup \mathrm{body}(B^{\perp}) &= \mathbb{R}^3.
\end{aligned}
$$

An example



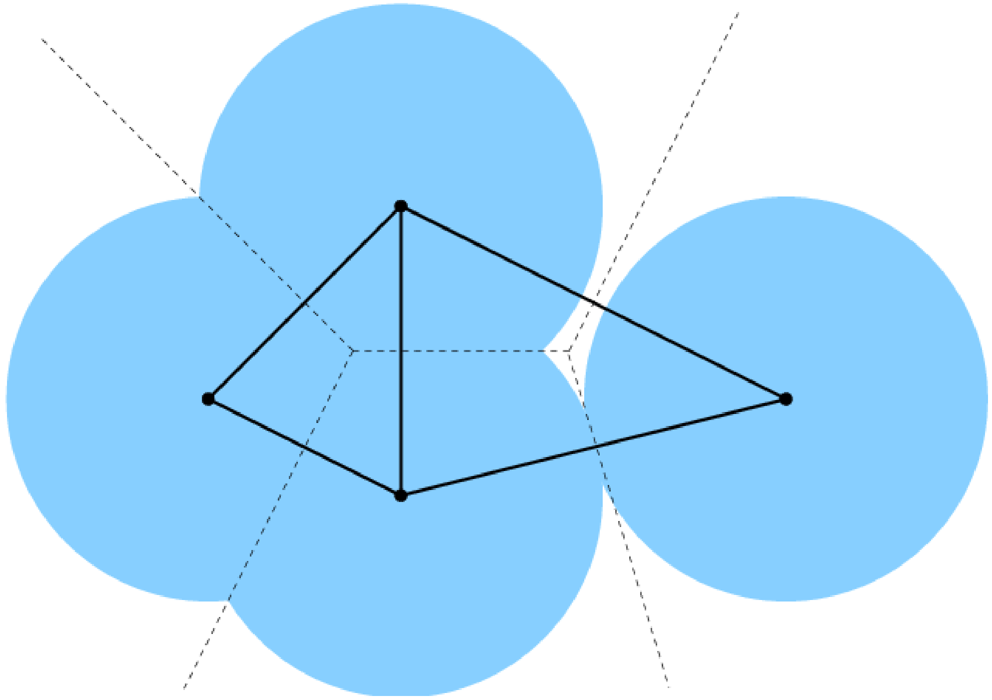
The molecular skin model of protein gramcidA. and a complementary portion

Skin Decomposition

Skin

- 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

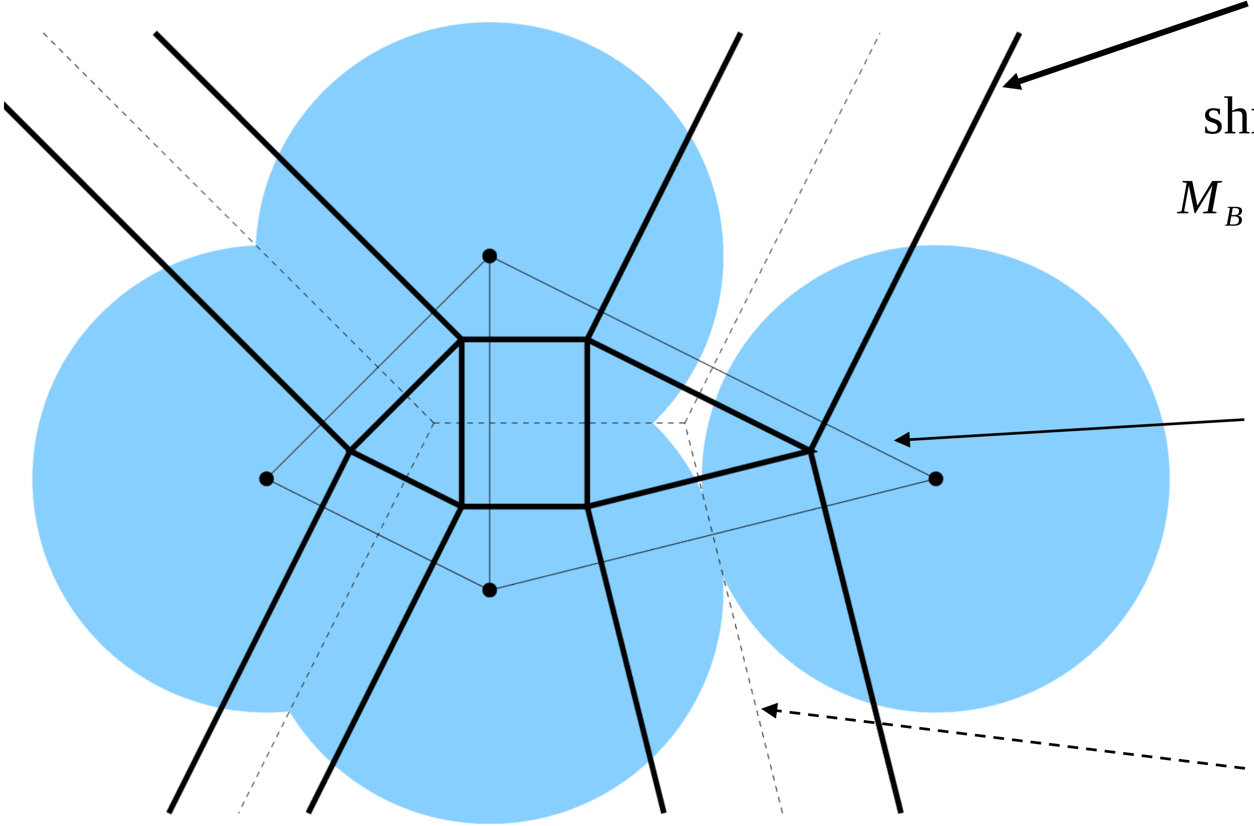
Weighted Delaunay Triangulation



Weighted Voronoi Diagram and Delaunay triangulation defined by 4 spheres in R^2

Mixed Complex

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



Mixed complex:

shrinking Minkowski sum

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

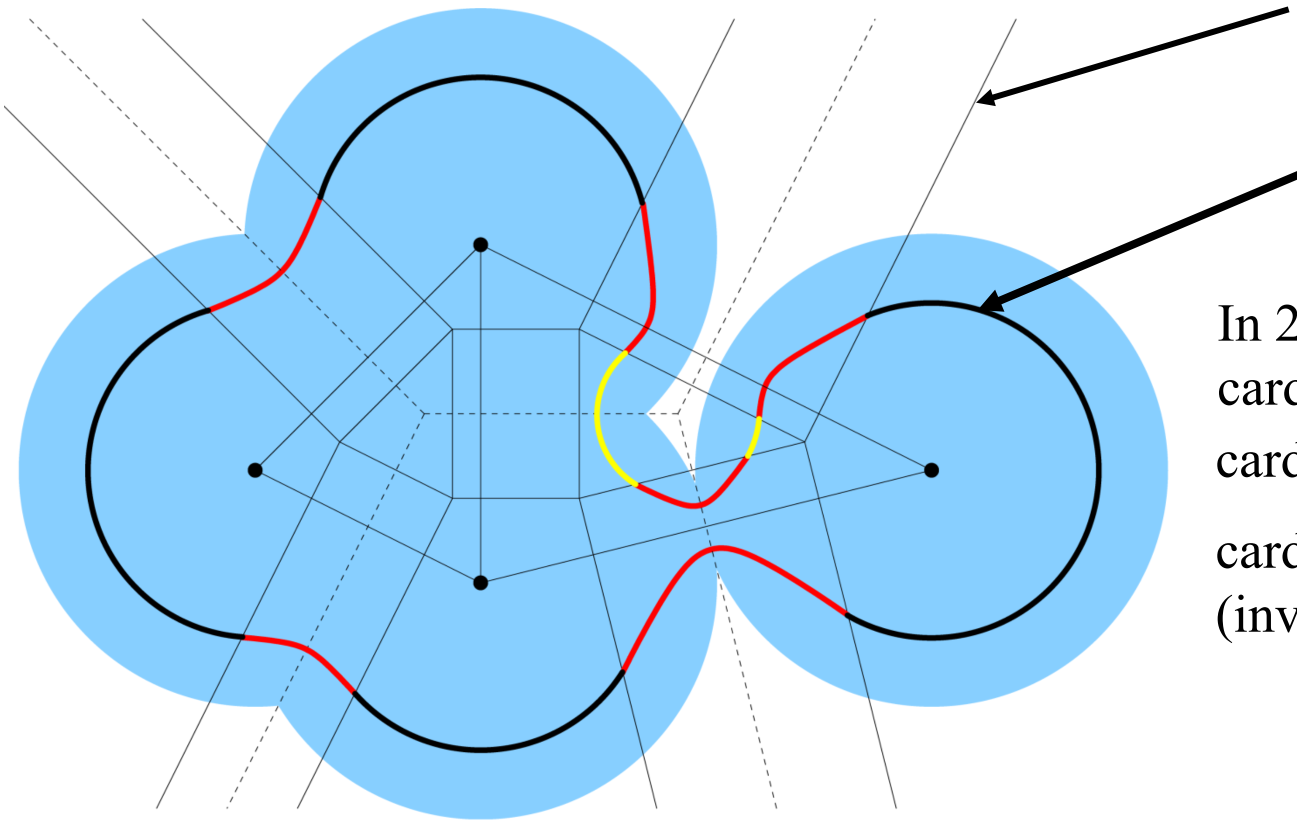
Weighted Delaunay triangulation D_B

Weighted Voronoi Diagram V_B

Skin decomposition

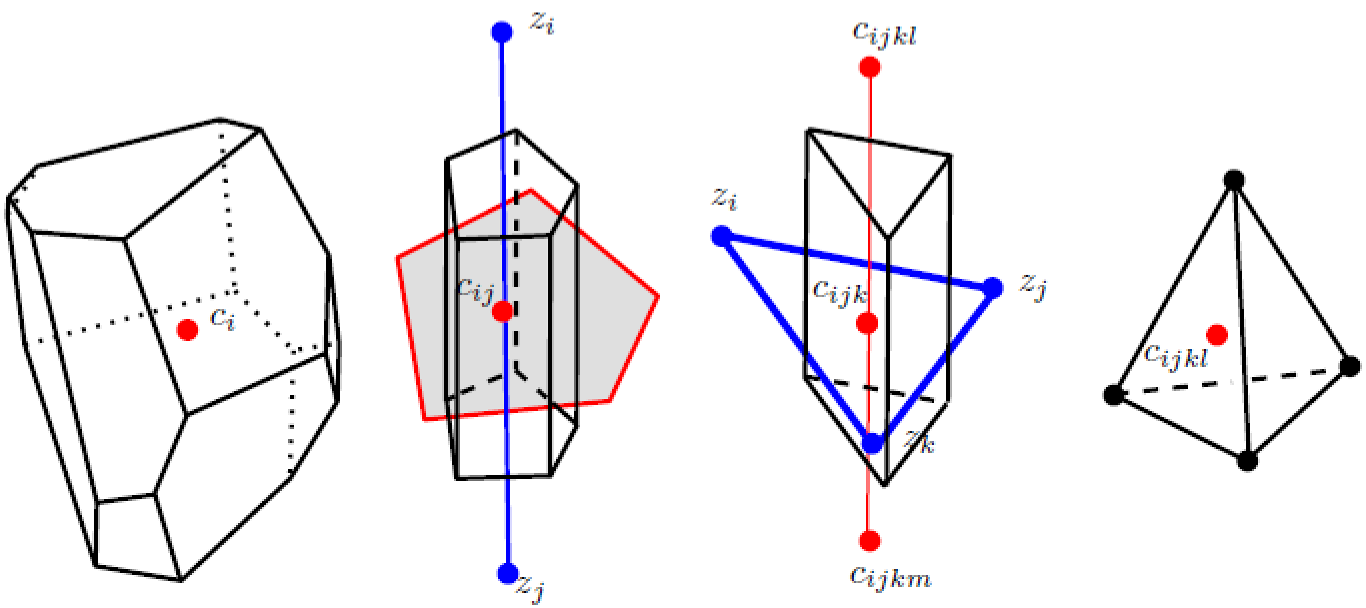
- The skin clipped in each mixed cell is quadratic

$$F_B \cap \mu_X = env(\sqrt{aff(X)}) \cap \mu_X$$

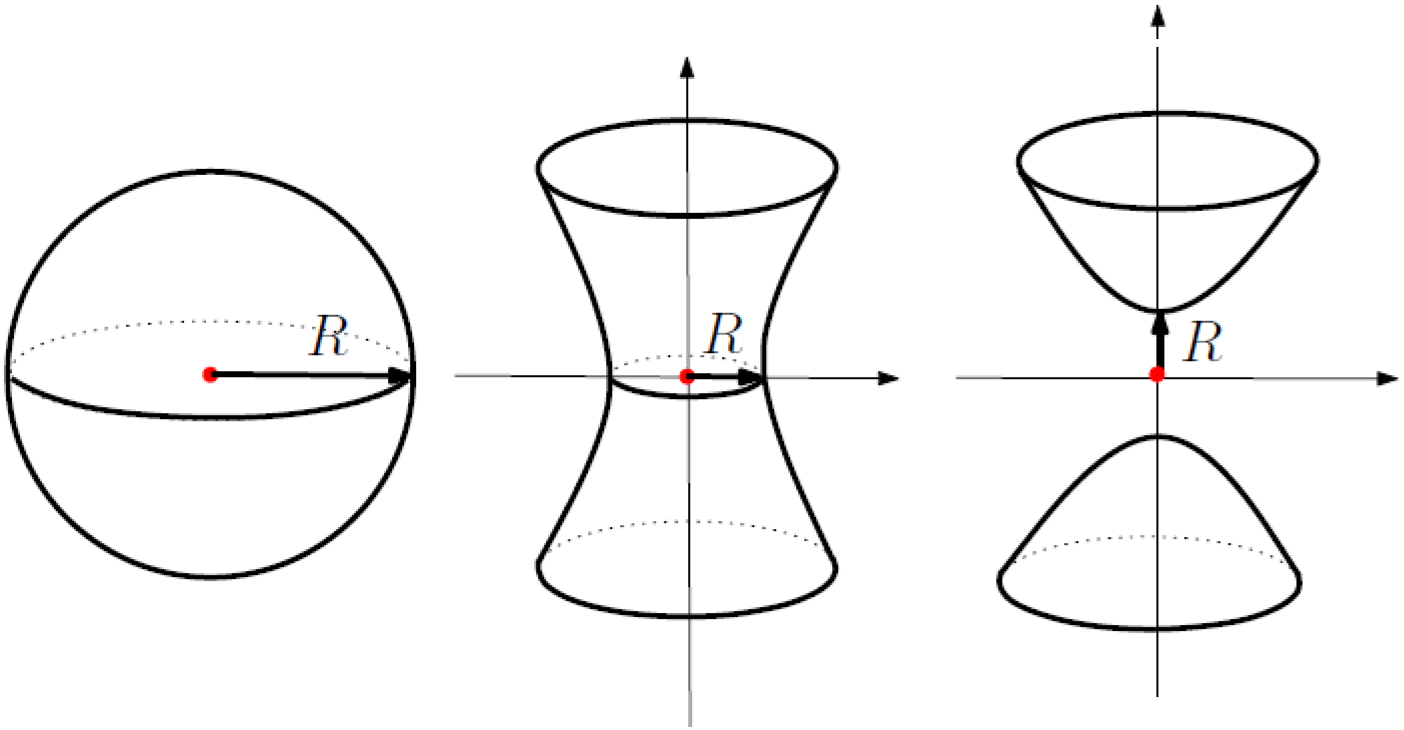


In 2 dimensions,
card(X) =1, sphere
card(X) =2, hyperbola
card(X) =3, sphere (inverse)

Mixed Cells in R^3



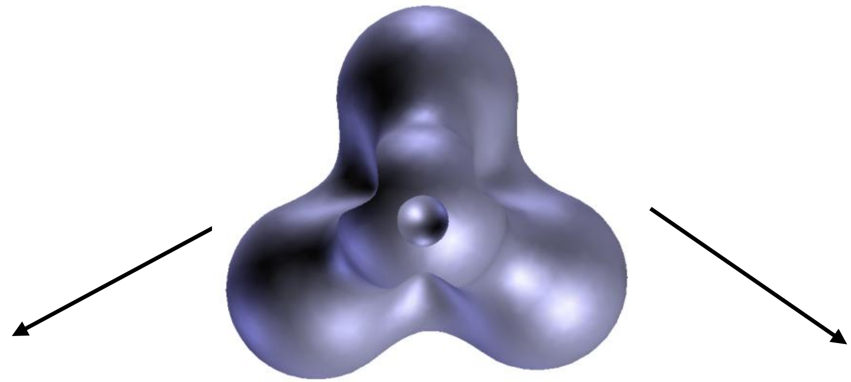
Quadratic Patches in R^3



Complexity

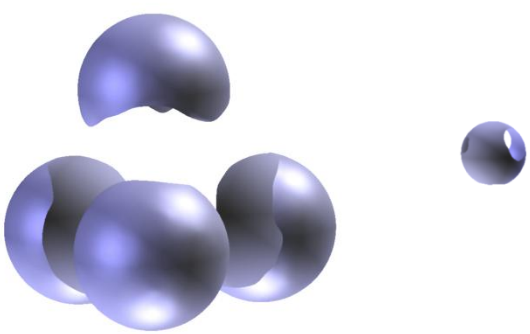
- Number of quadratic patches in the skin surface specified by n spheres can $O(n^2)$
- For molecules, the number of patches is usually linear to the number of atoms

Three dimensional example

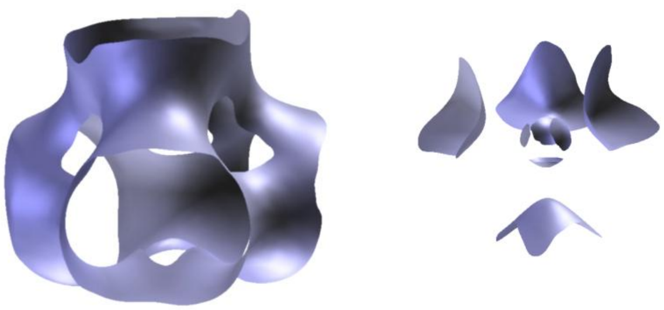


Sphere patches

Hyperboloid patches

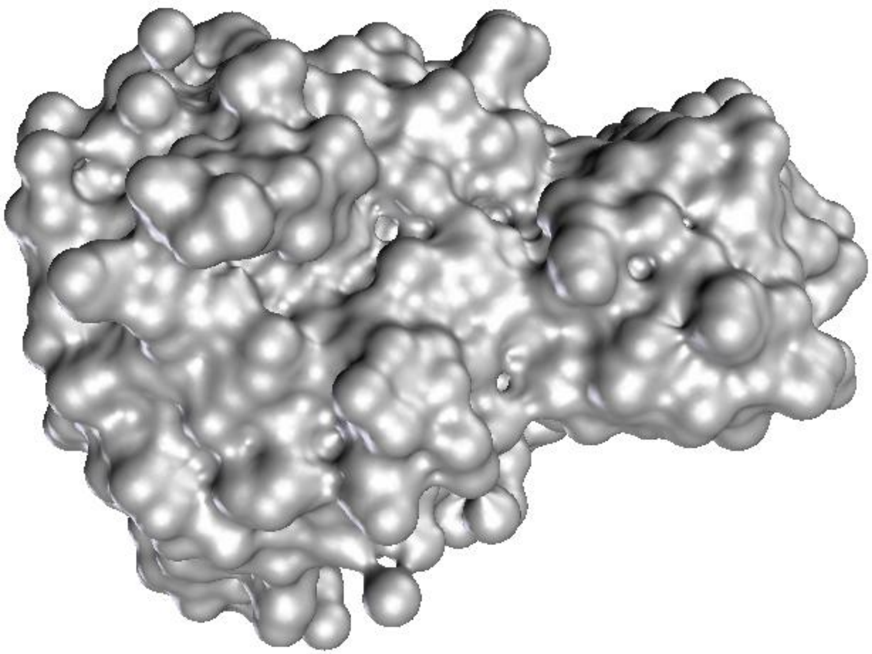


card(X) =1, 4



card(X) =2, 3

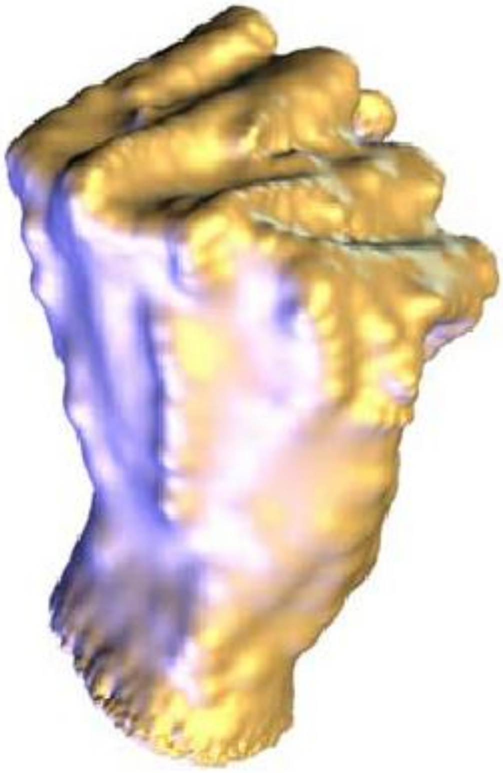
Skin surfaces

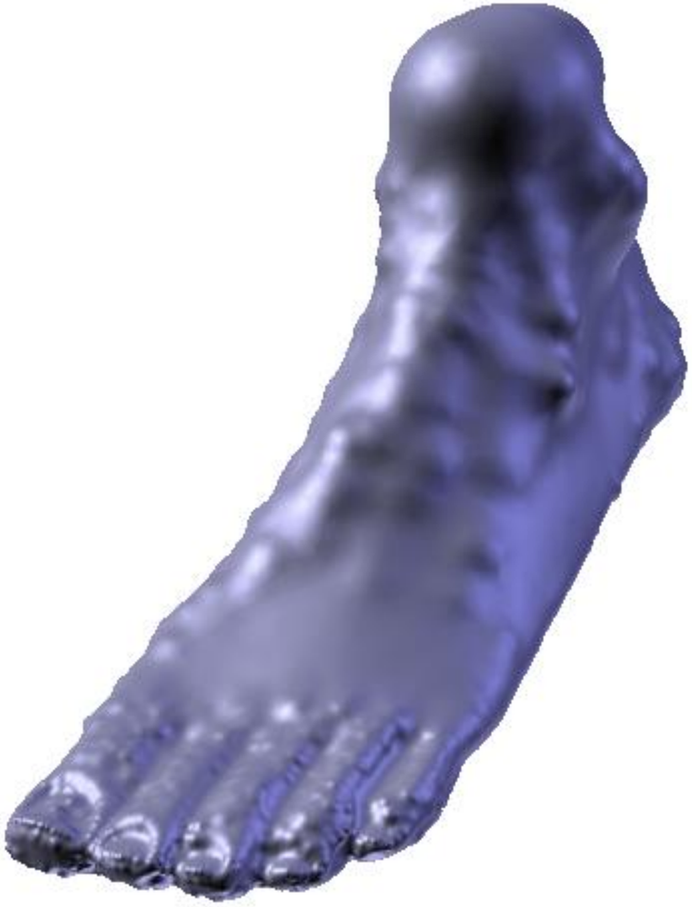


A protein

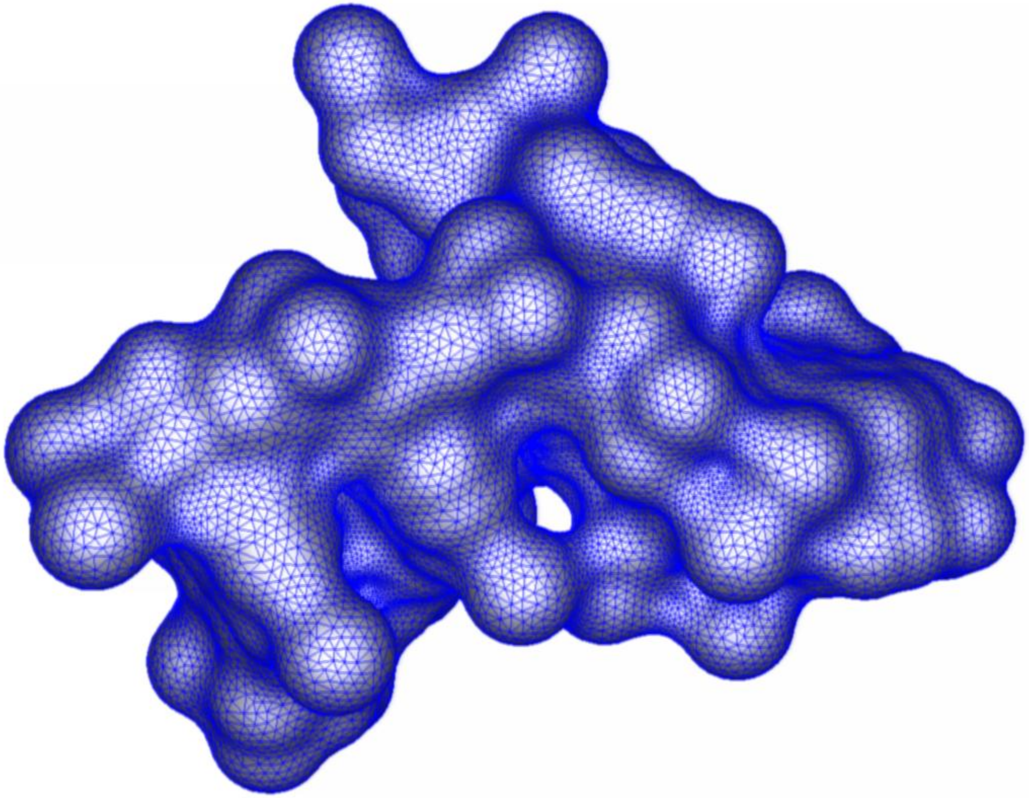
Face model

Skin surfaces





Adaptive Meshing

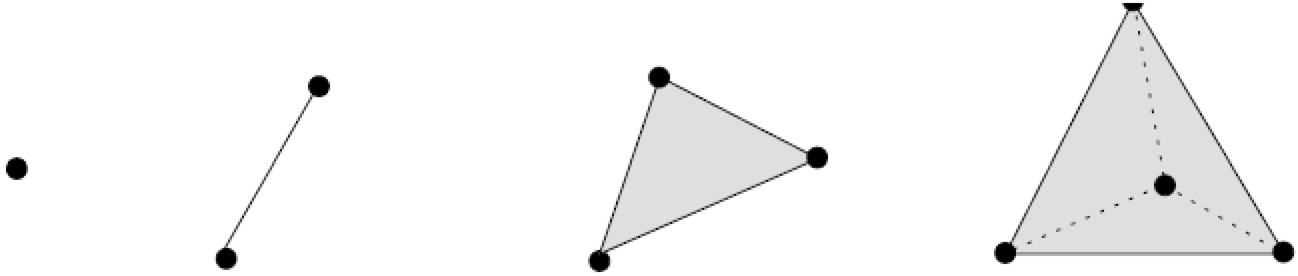


Meshing

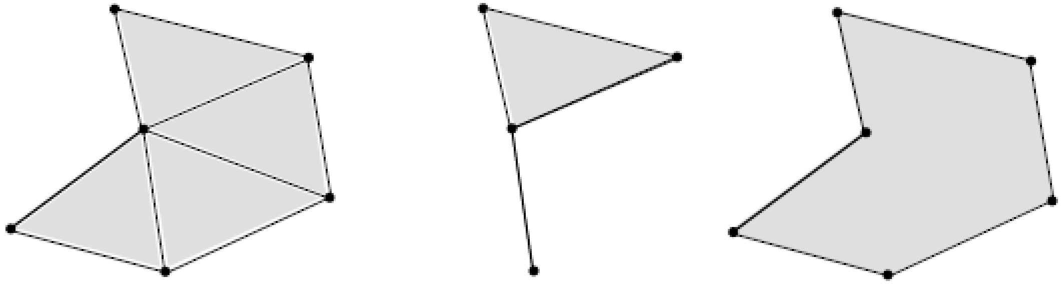
- A meshing, or triangulation of a surface *F* is a **simplicial complex** whose underlying space is **homemorphic** to F.
- Geometry preserved
  - Hausdorff distance between the surface and mesh has a upper bound
- High mesh quality.
  - The smallest angle of the mesh has a lower bound

Simplicial Complex

- Simplex

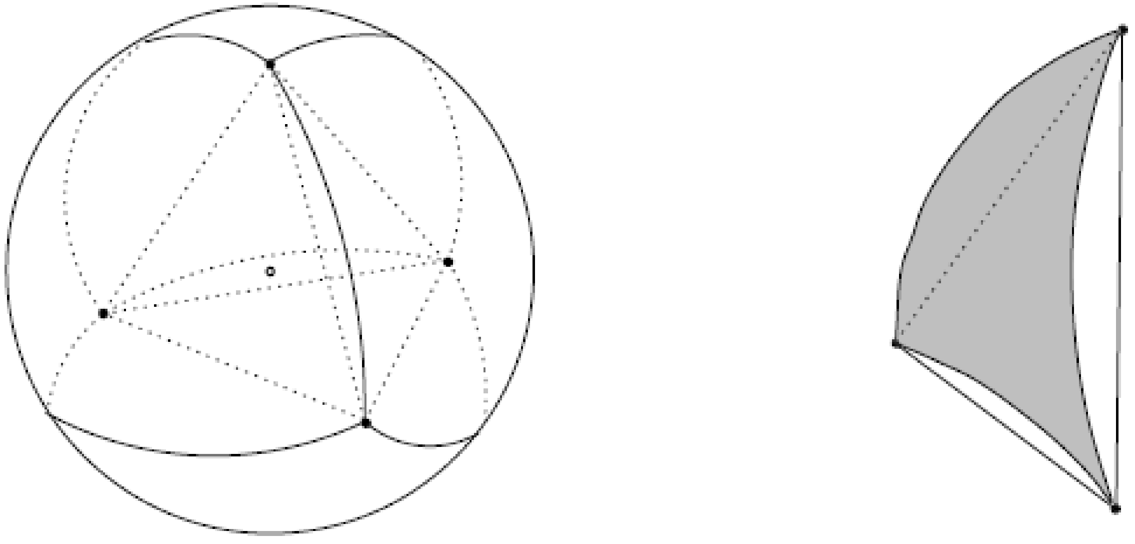


- Simplicial complex and its underlying space



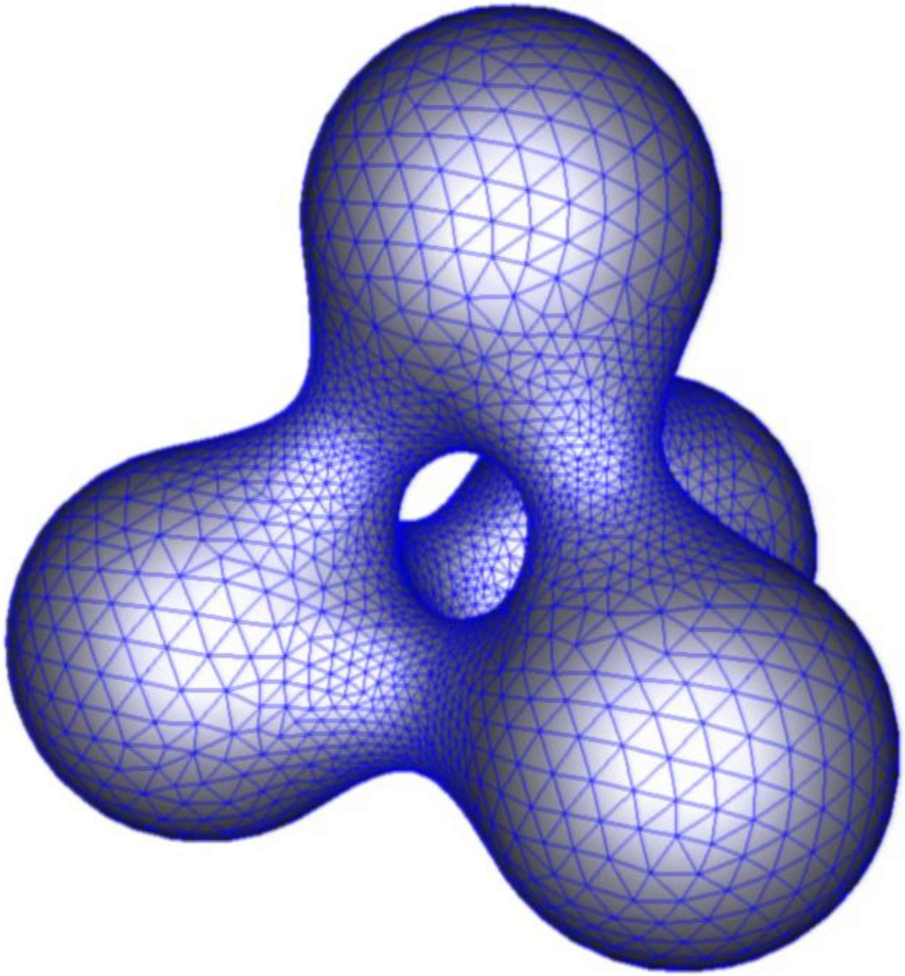
Homeomorphism

- A map *f* is a homeomorphism if it is bijective and has a continuous inverse



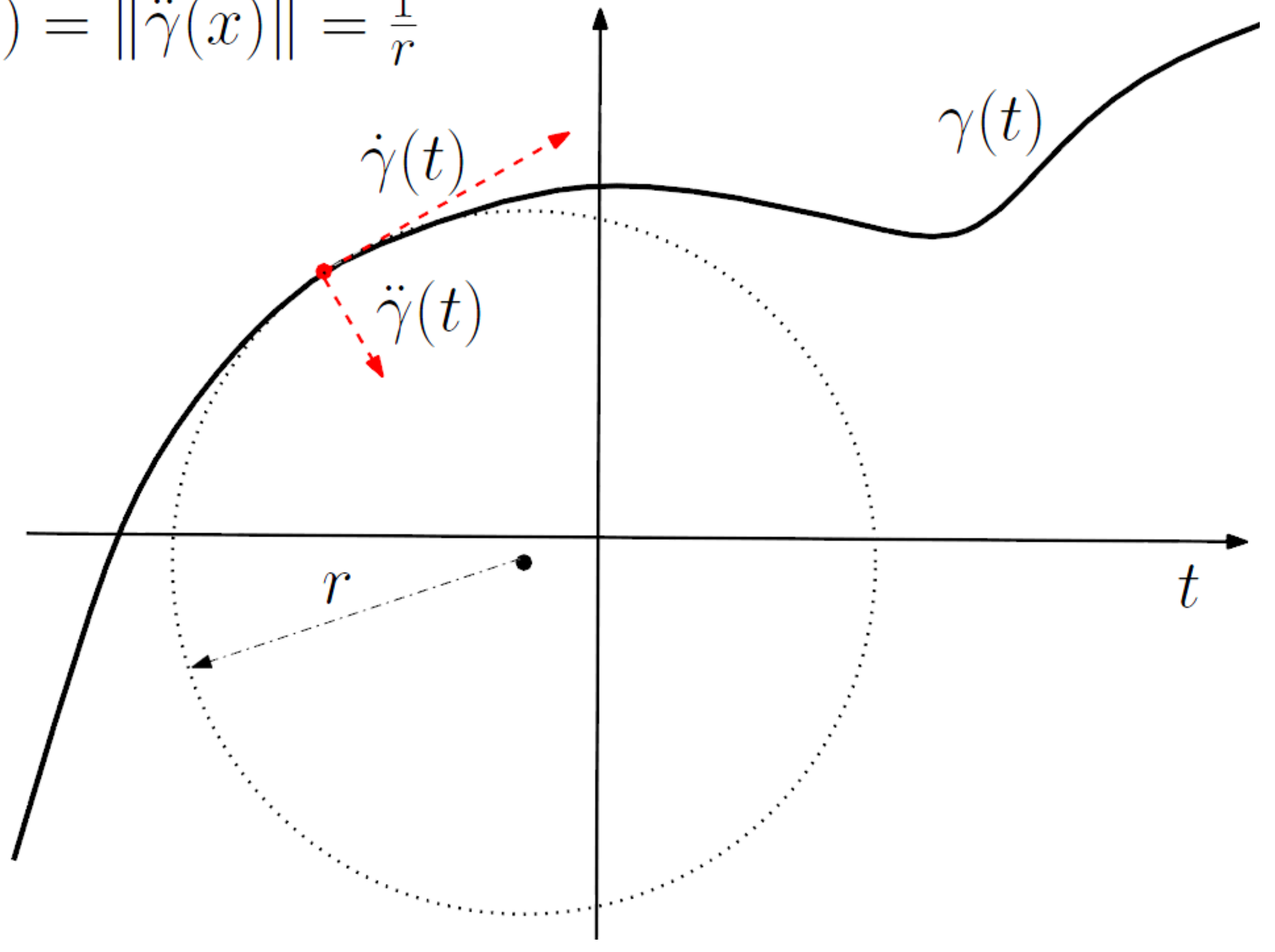
Adaptive

- Triangle size in the adapts the local surface geometry



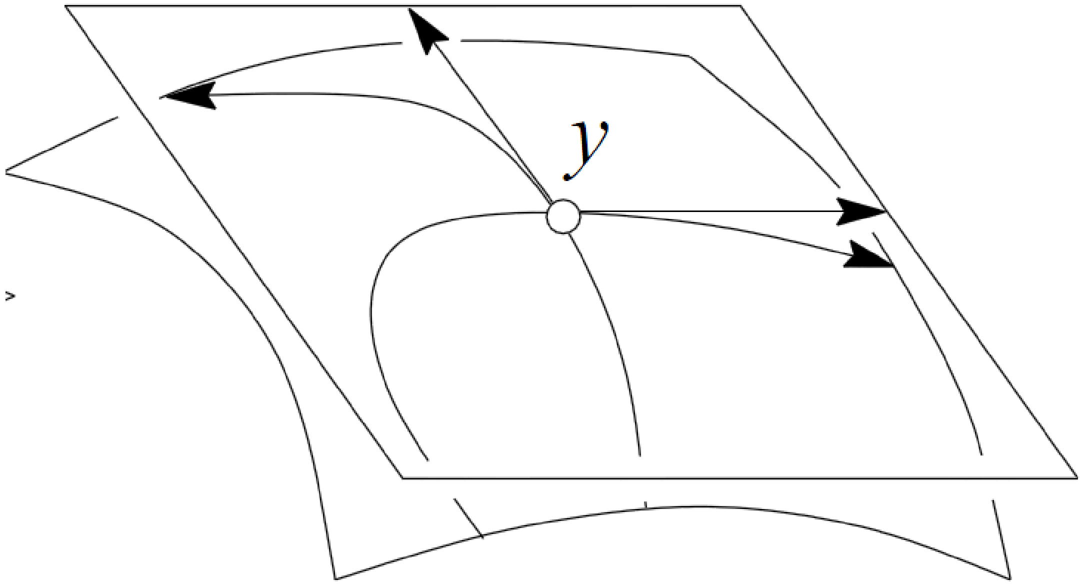
Curvature--Plane curves

$\kappa(x) = \|\ddot{\gamma}(x)\| = \frac{1}{r}$



Surface curvature

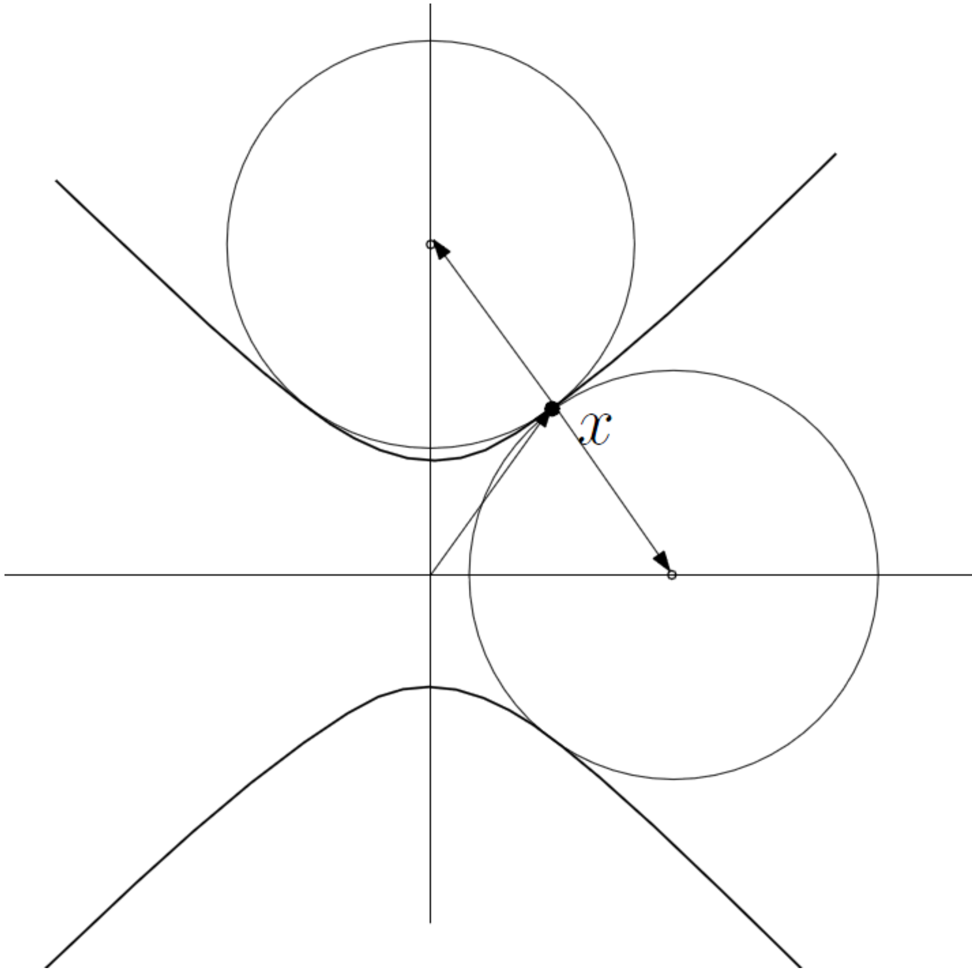
- Principle Normal Curvature



- Euler's formula (1760)

Curvature of skin surface

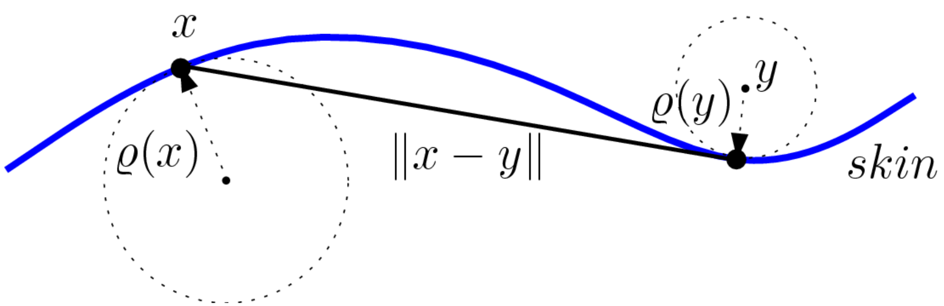
- Constant curvature (1/R) on spherical patches
- On a hyperboloid, the maximum more curvature is 1 over the radius of sandwiching sphere



Curvature variation

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

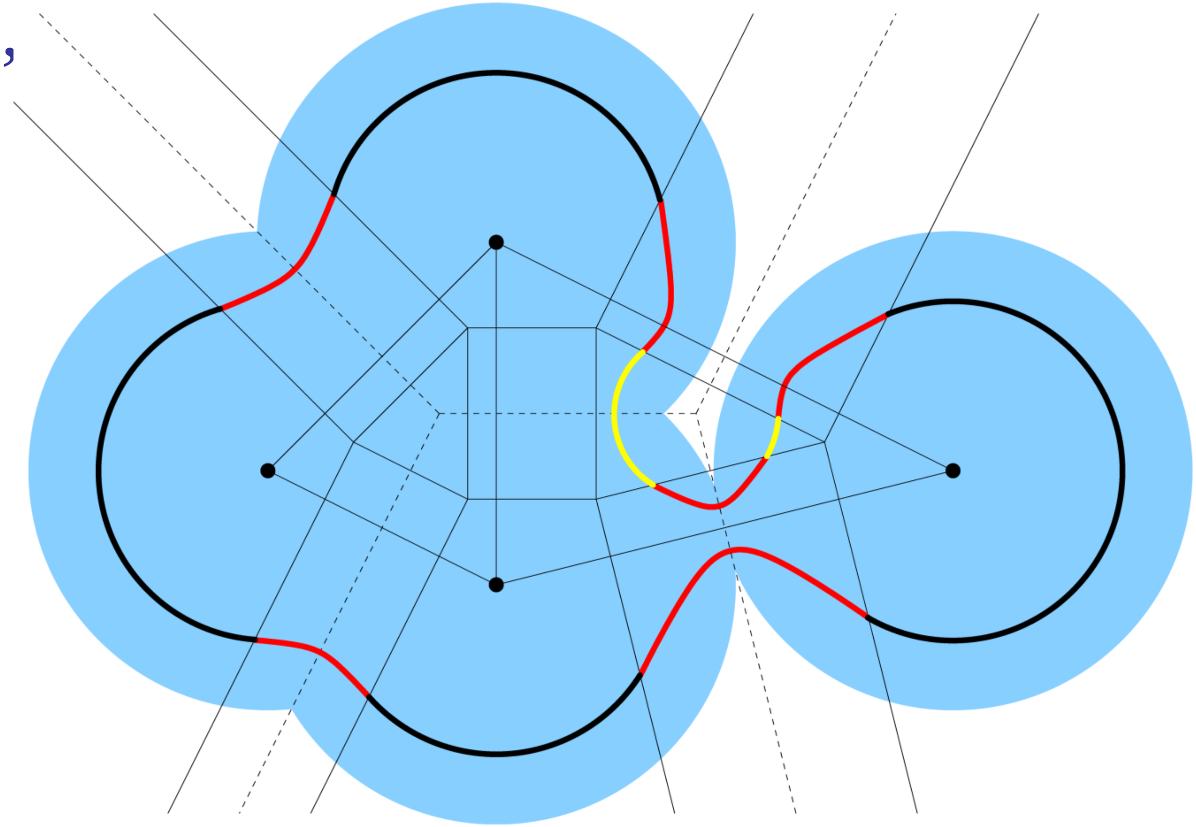
$$|\varrho(x) - \varrho(y)| \leq \|x - y\|.$$



- This property implies that the curvature varies slowly on the surface.

Local length scale

- The local length scale at a point *x* on the skin surface is the lower bound of the local feature size *lfz(x)*,

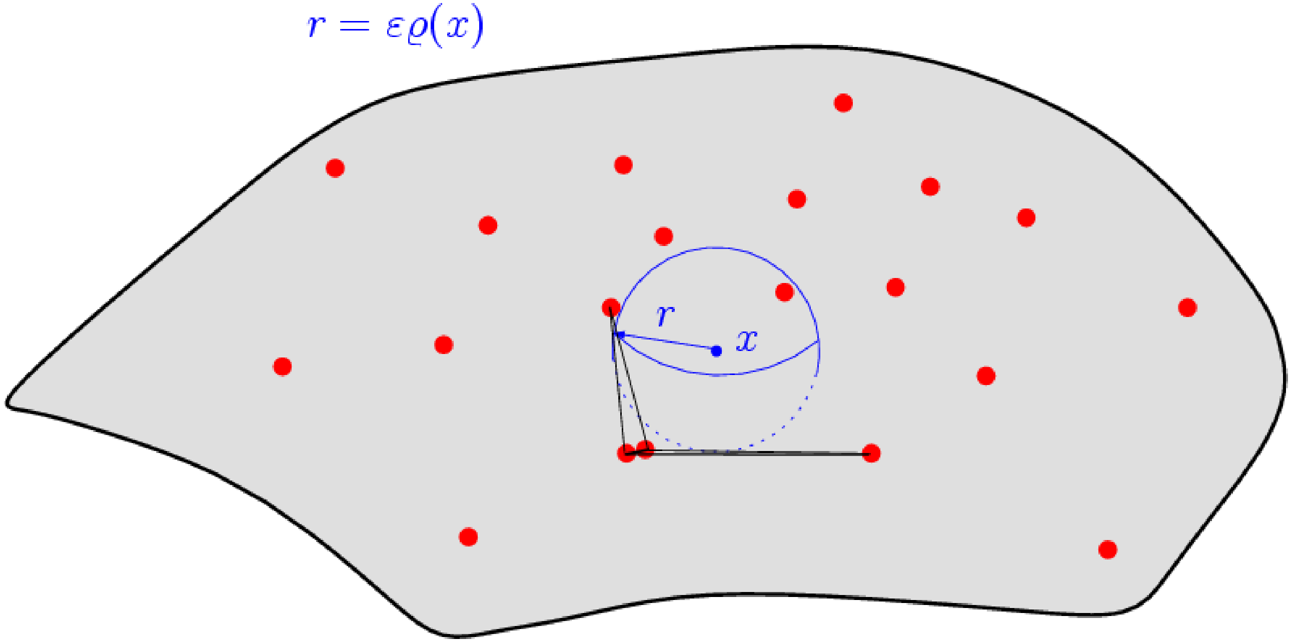


Adaptive Meshing

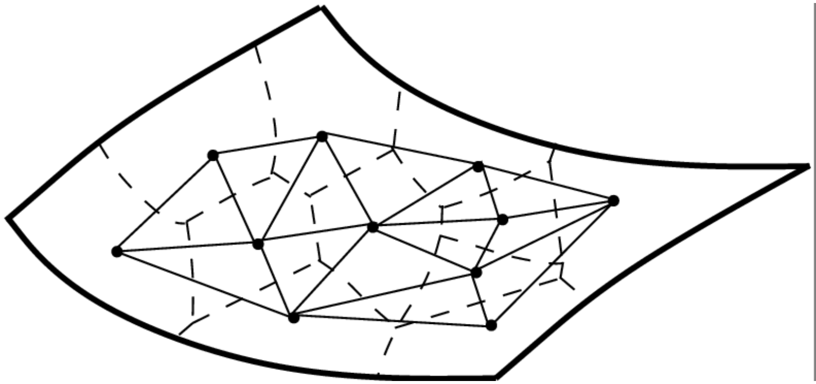
- Generation of an adaptive sampling.
- Construct a triangulation using the samples.

ε-sampling of the Skin Surface

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



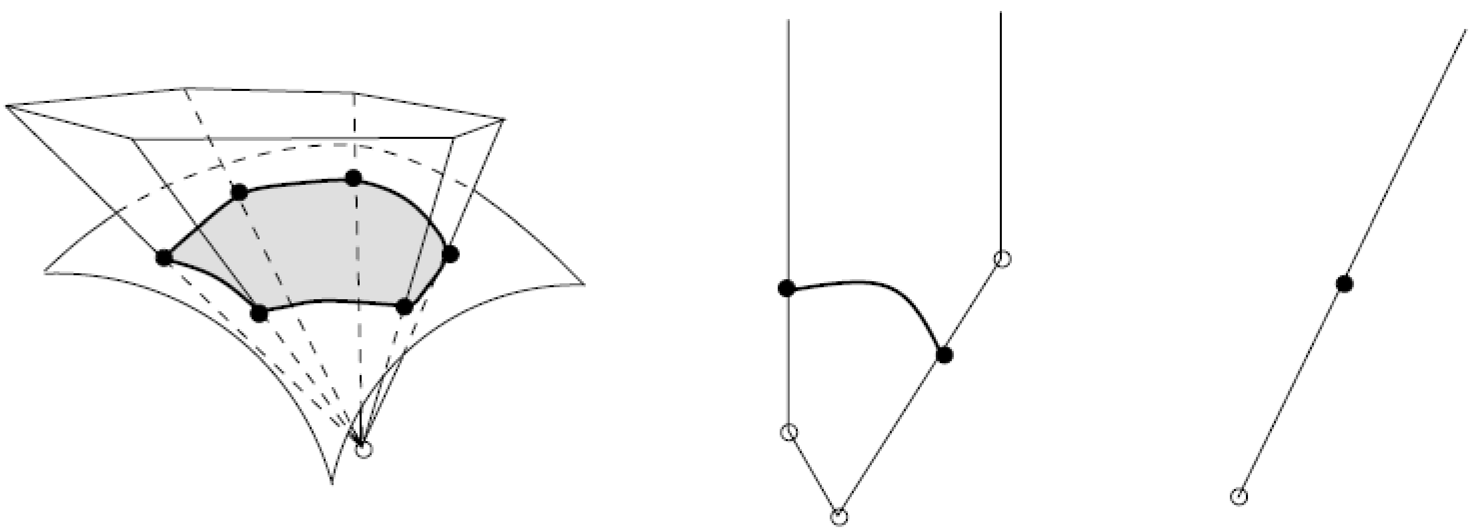
Restricted Delaunay triangulation



- A set of points $T \subseteq F_B$
- Restricted Voronoi polygon of $a \in T$
  $\upsilon_a' = \upsilon_a \cap F_B$
- Restricted Voronoi Diagram $V_T = \bigcup \upsilon_a', a \in T, \nu_a' \neq \phi$
- Restricted Delaunay triangulation D_T' of F_B is the dual of V_T

Homeomorphism Theorem

- Closed Ball Property

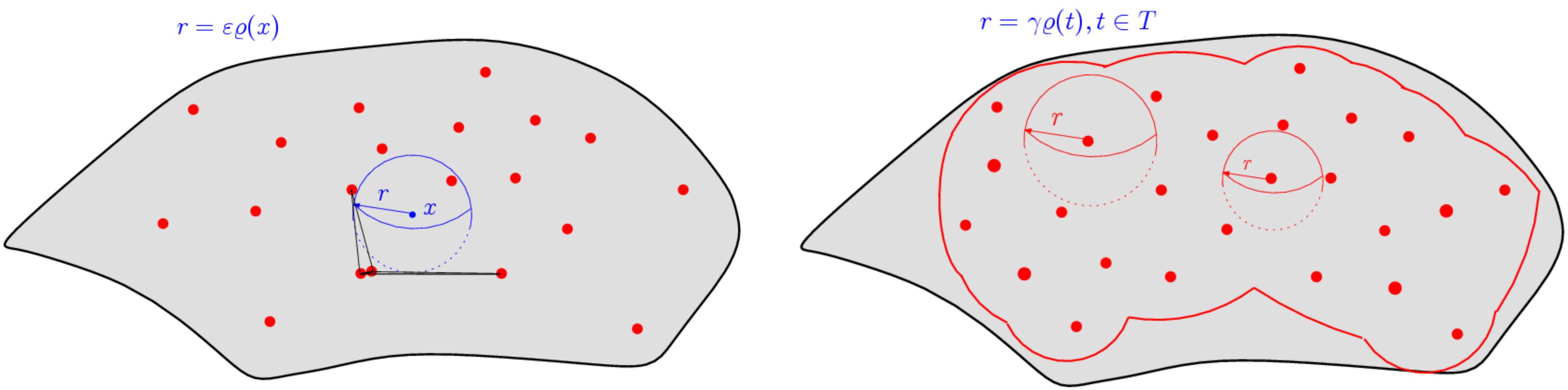


ε need to be small

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

Even ε-sampling

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



Skin Meshing using Restricted Union of Balls

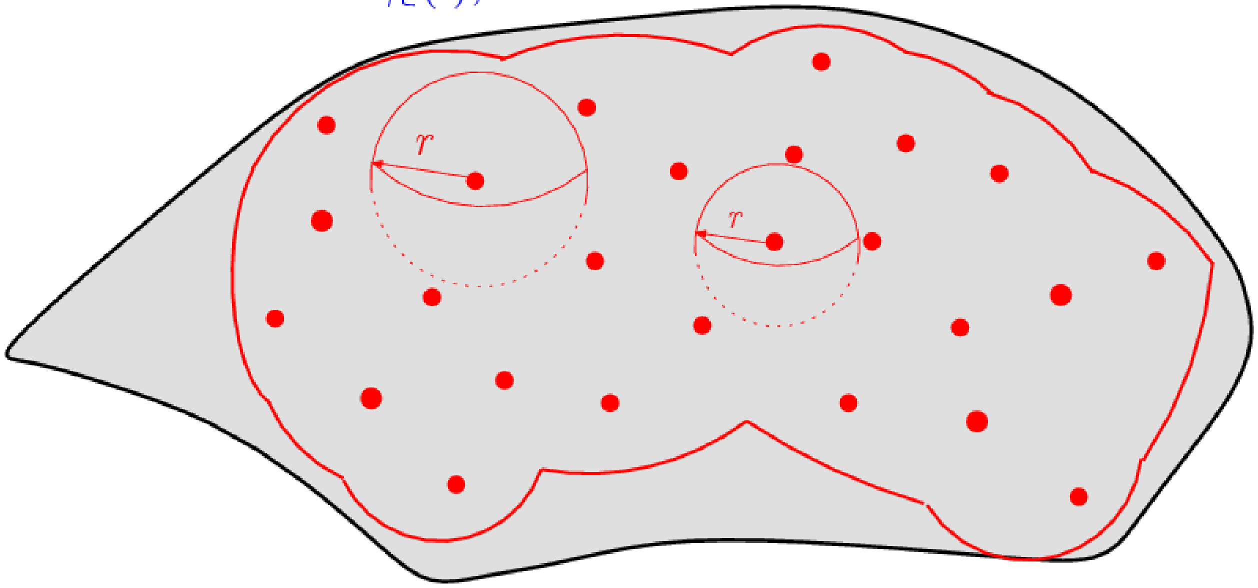
Overview of the algorithm

- Generate an even ε-sampling incrementally
- Construct the Delaunay triangulation of the sample points simultaneously
- Extract the restricted Delaunay triangulation as the surface mesh

Even ε-sampling

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

$r = \gamma\varrho(t), t \in T$



Observation

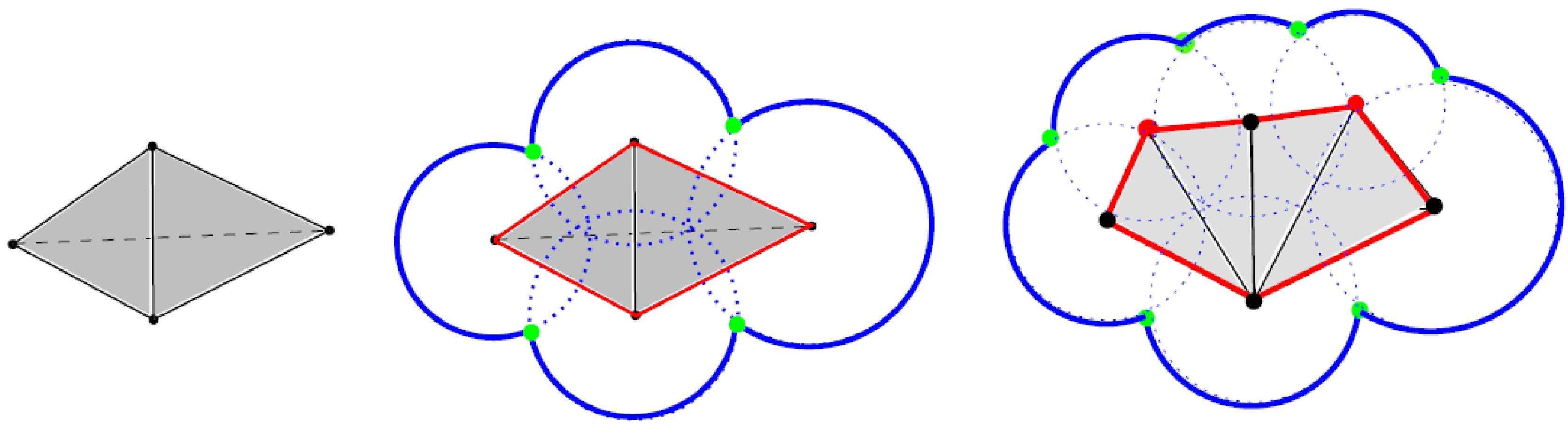
- If the restricted union of balls covers the whole surface with some feasible *r* value, the RDT of the sample points is homeomorphic to the surface and has a lower bound on its minimum angle.

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^o *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

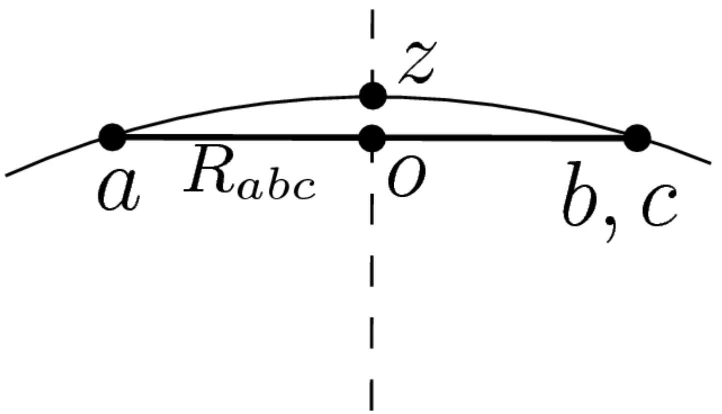
- Small radius property

$$R_{abc} < \frac{\varepsilon}{1-\varepsilon}\varrho_{abc}.$$

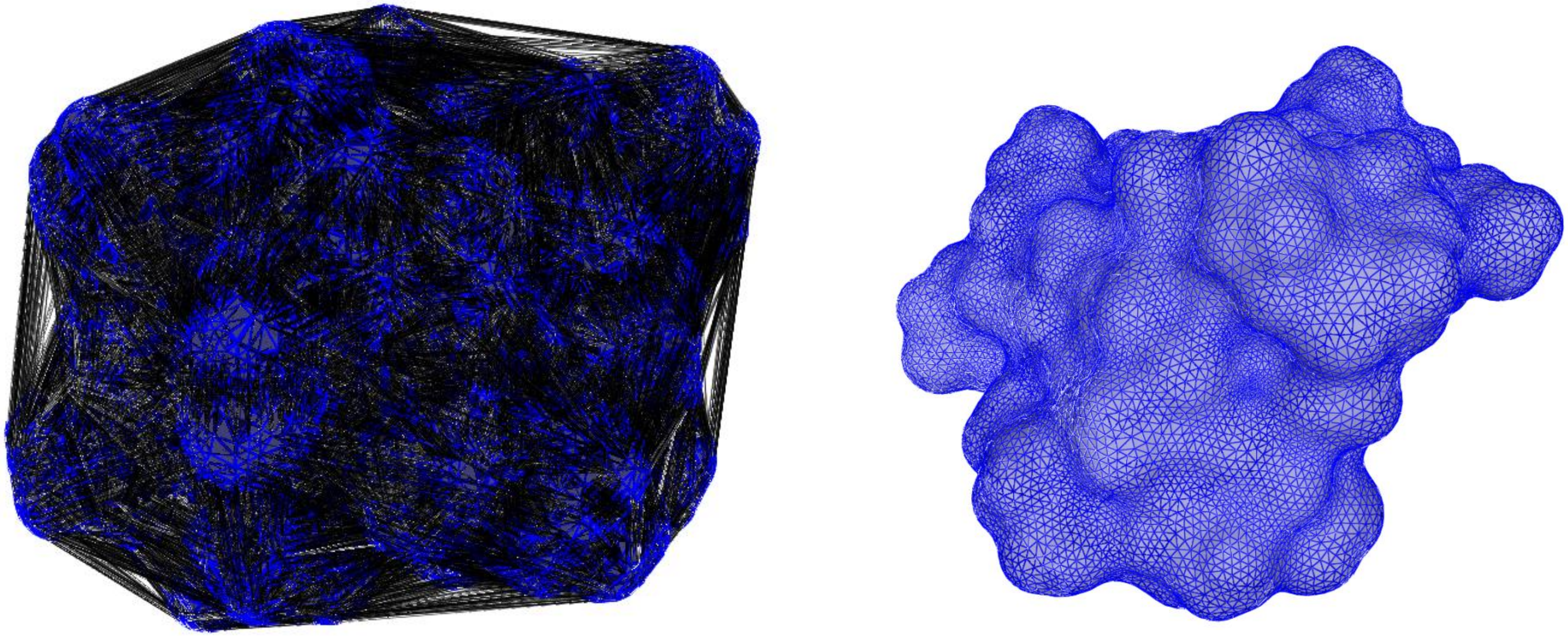
- Restricted Delauany property

$$\|oz\| \leq \frac{\varepsilon^2}{2}\varrho_{abc},$$

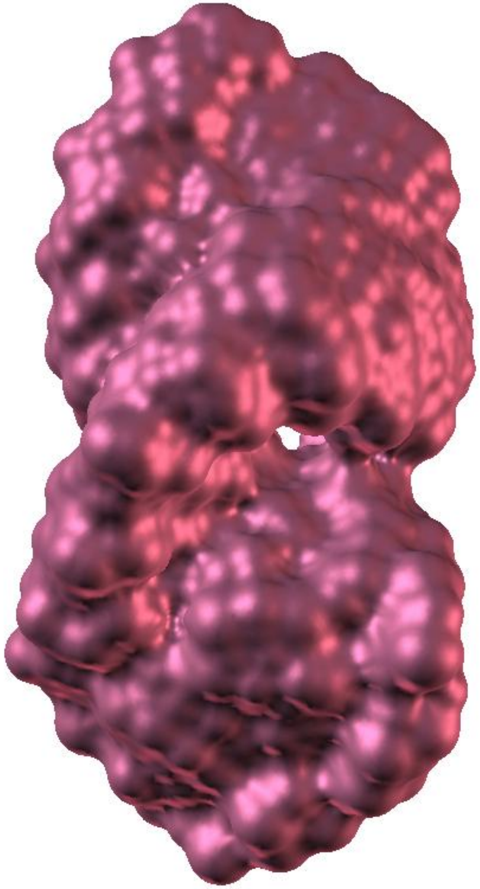
$$\varrho_{abc} = \min\{\varrho(a), \varrho(b), \varrho(c)\}$$

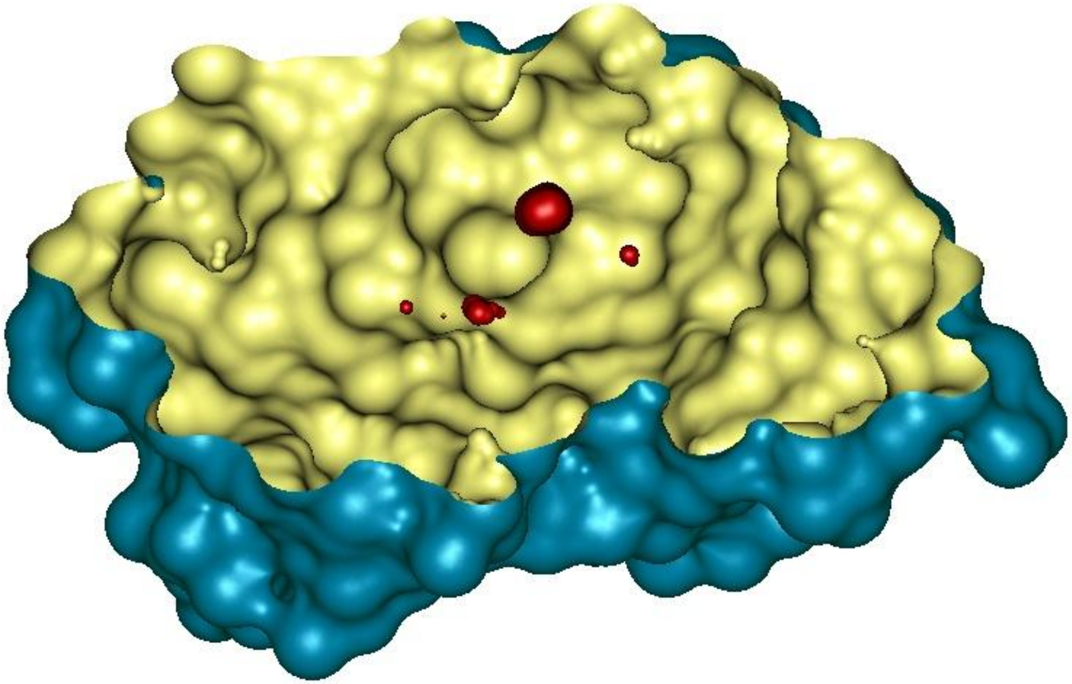


Surface Mesh

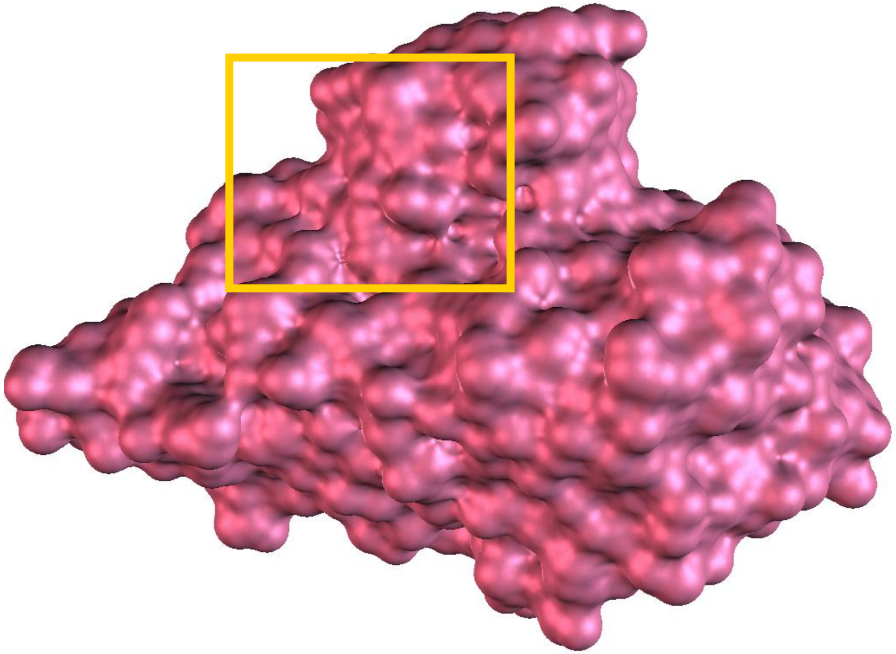


More examples

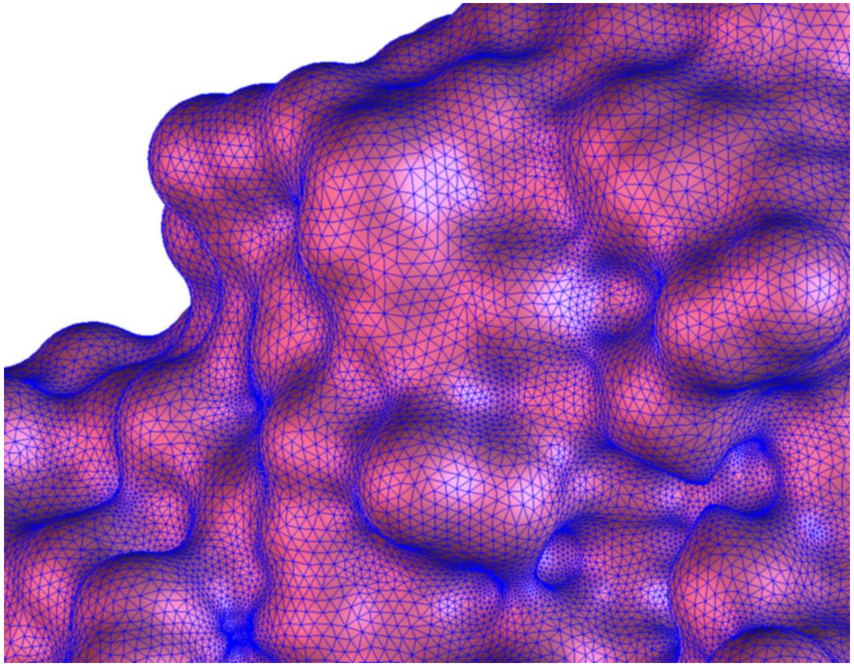




Mesh Quality



Skin model for a protein



Quality statistics

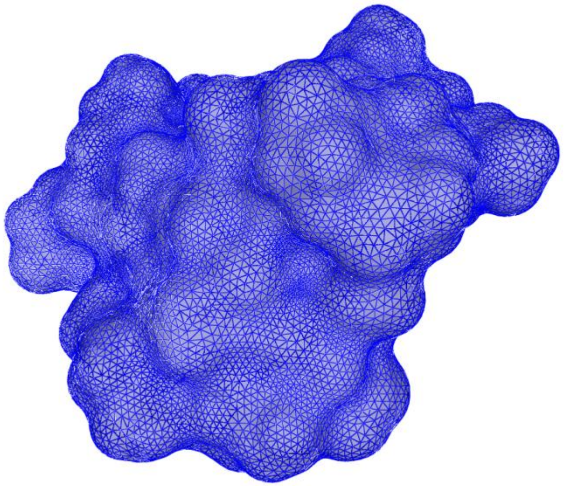
molecular name	no. triangles in the mesh	minimum angle distribution(%)			
		50°-60°	30°-50°	20°-30°	Less than 20°
Helix	98,017	58.21	41.56	0.23	0
*HIV*2	226,758	56.22	43.54	0.24	0
1*CHO*	253,024	56.00	43.77	0.22	0.01
1*ACB*	290,476	56.20	43.56	0.2397	0.0003

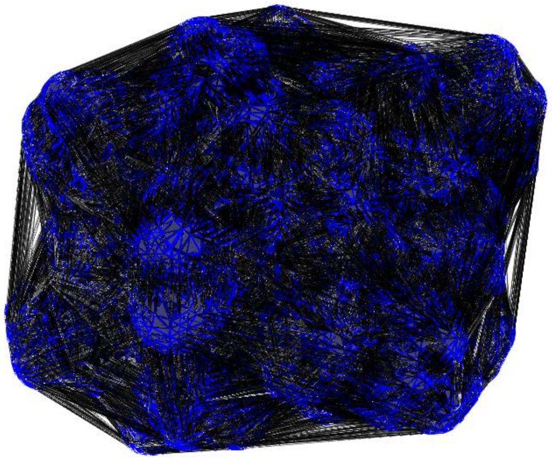
Table 4.2: Triangle quality distribution.

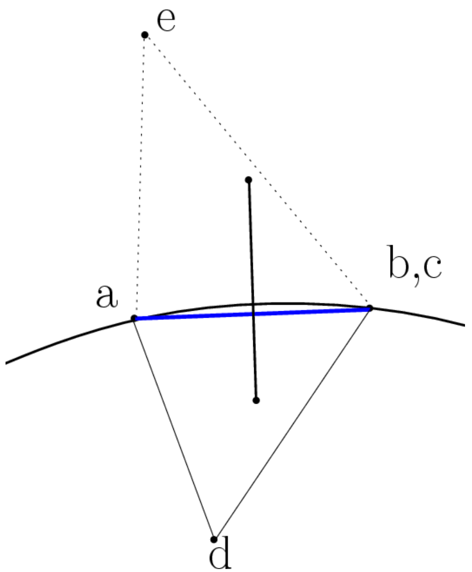
Tetrahedral Meshes

Initial Tetrahedralization

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

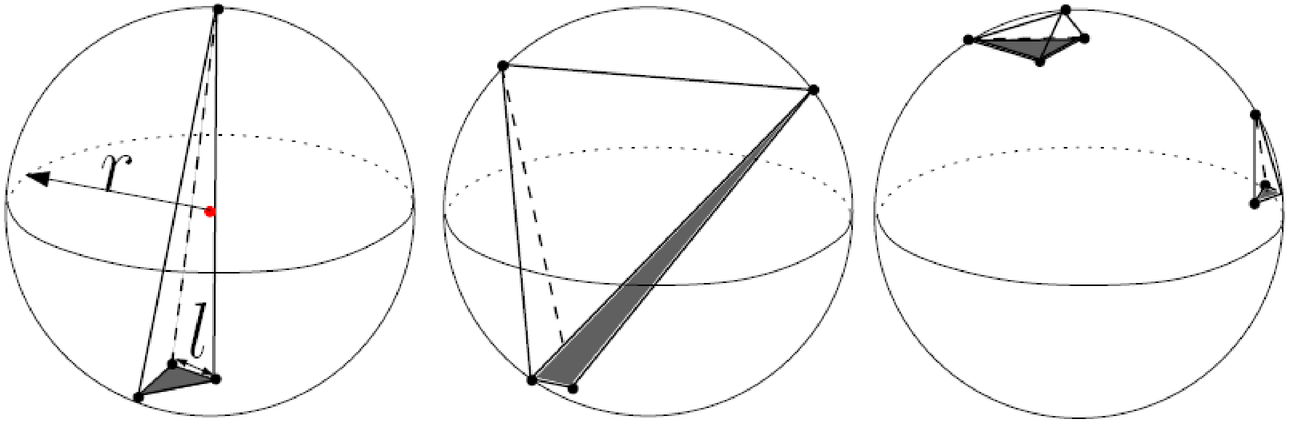






Tetrahedral Quality

- Radius-edge ratio

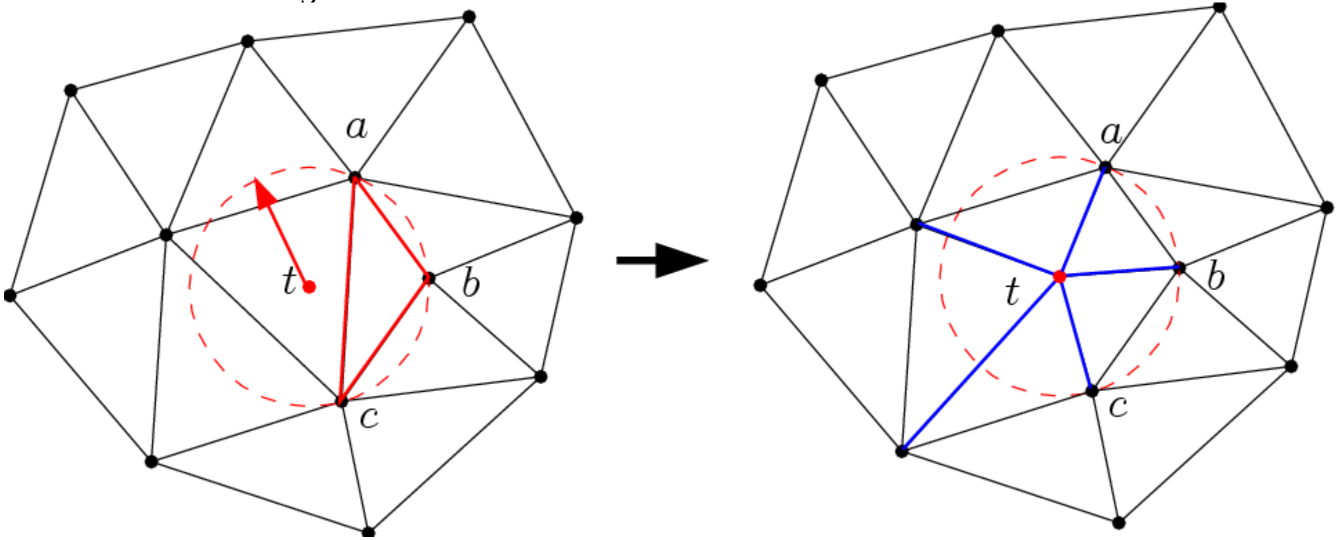


(a) (b) (c)

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

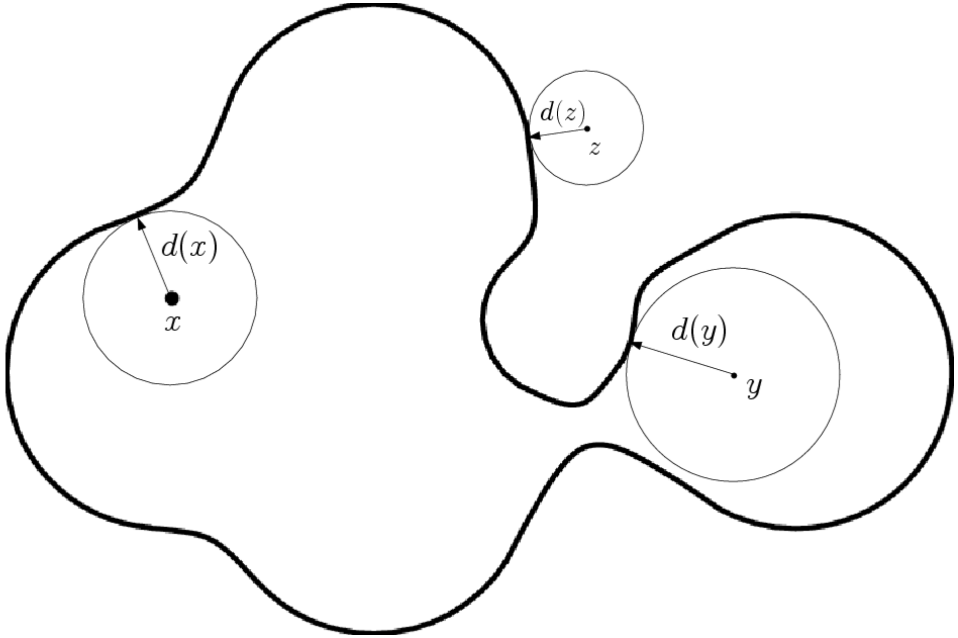
Prioritized Delaunay Refinement

- 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.

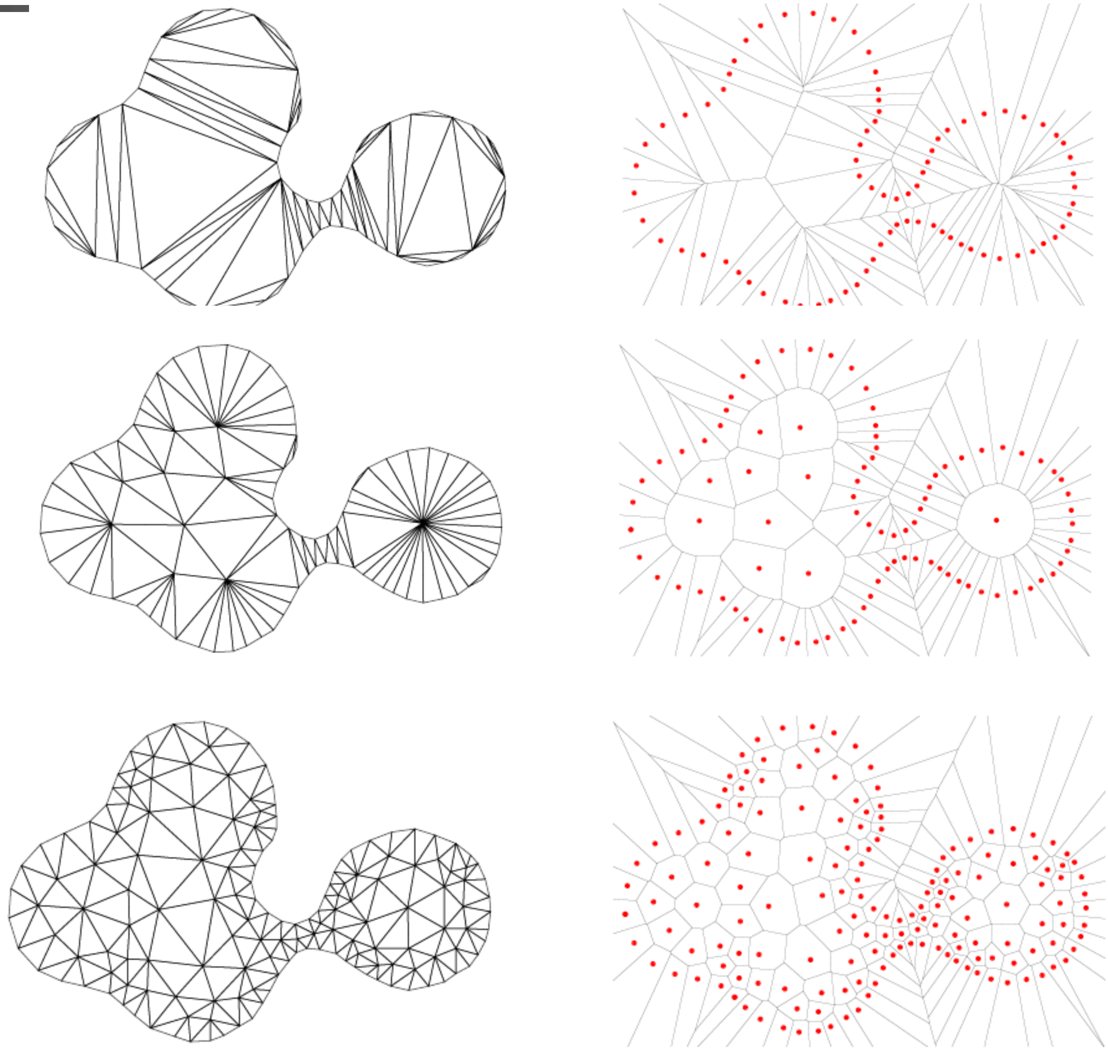
Prioritized Delaunay Refinement

- Distance function

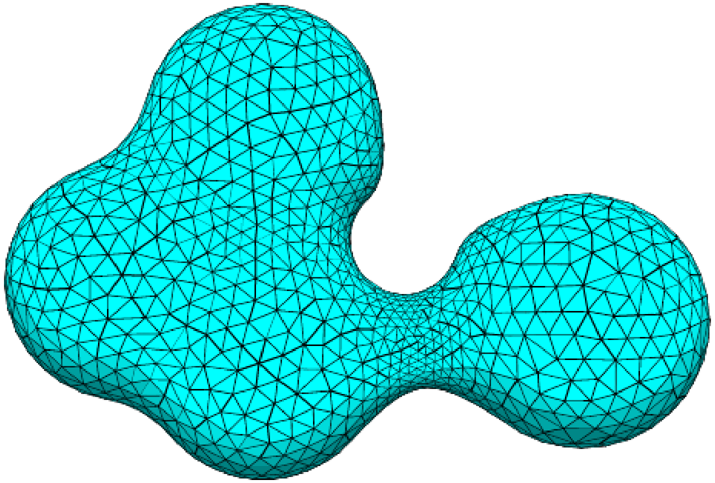
$$d(x) = \inf_{p \in F_B} \|x - p\|, \forall x \in \mathbb{R}^3.$$

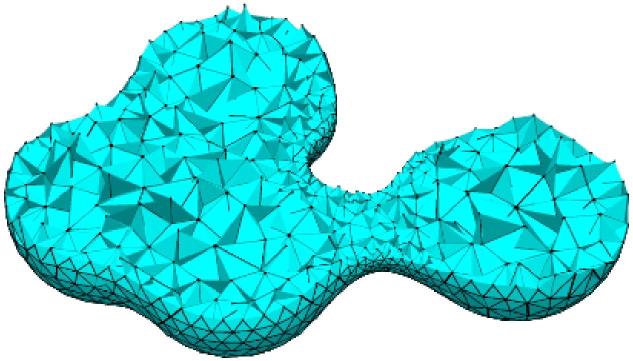


Prioritized Delaunay Refinement

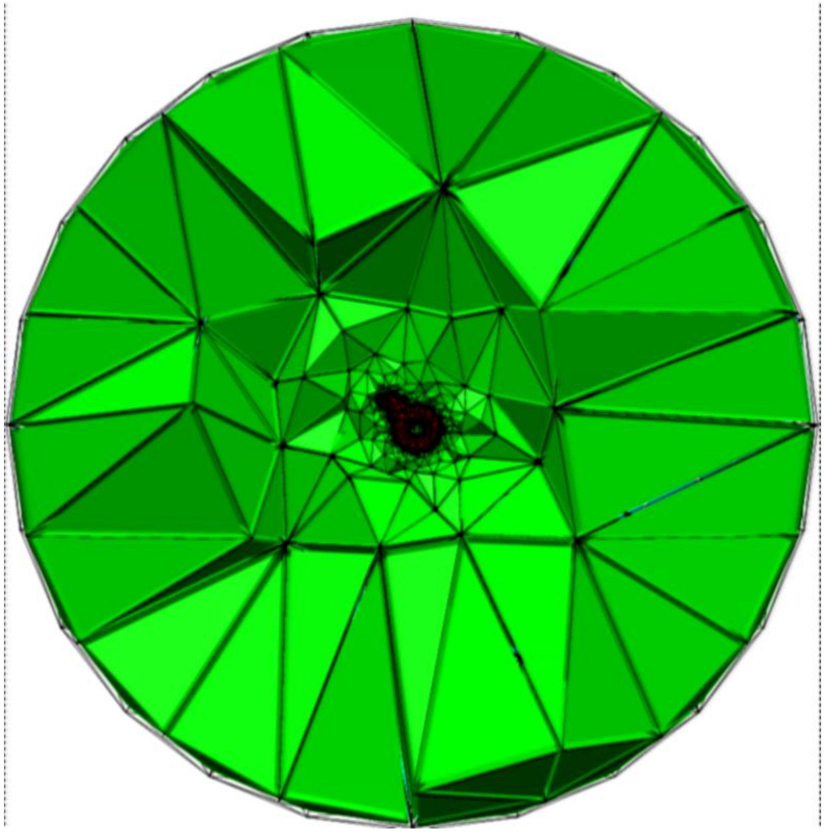


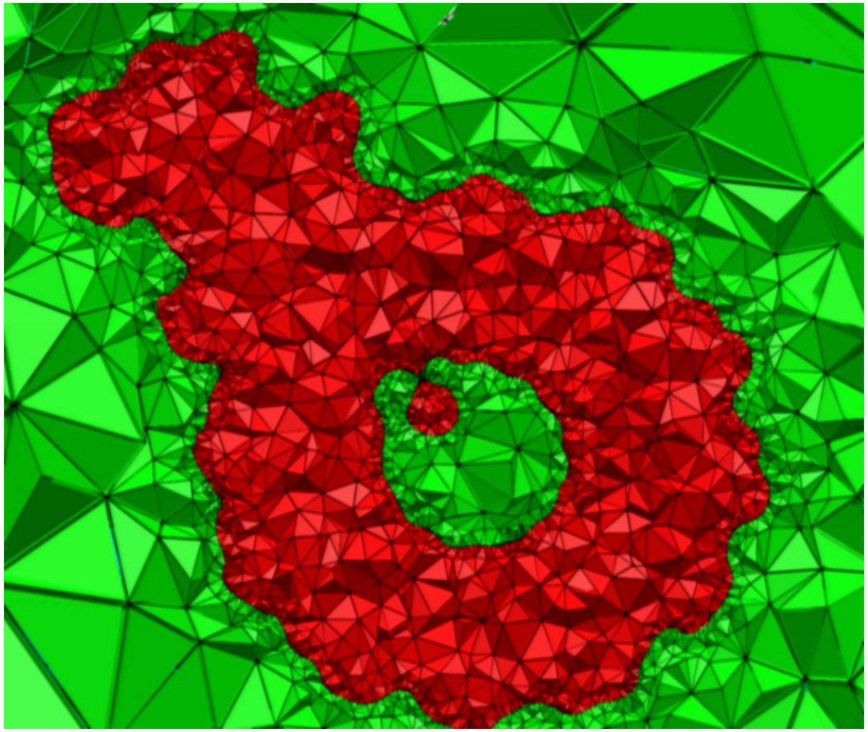
An examples





Results



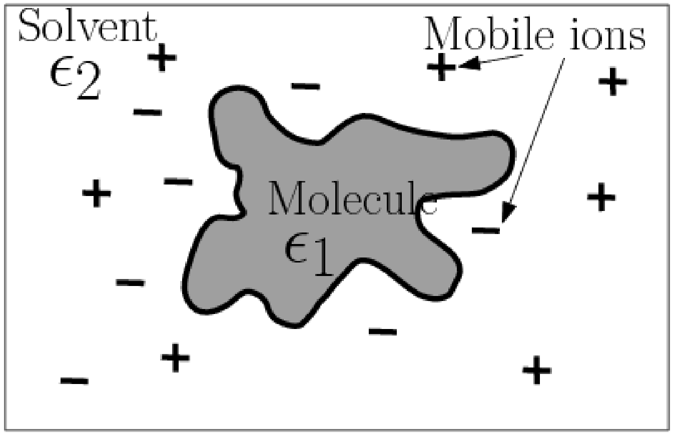


Calculating Molecular Electrostatics

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

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

$$\nabla^2\phi_2(x)) = \kappa^2\frac{k_BT}{e_c}\sinh(\frac{e_c\phi_2(x)}{k_BT})$$



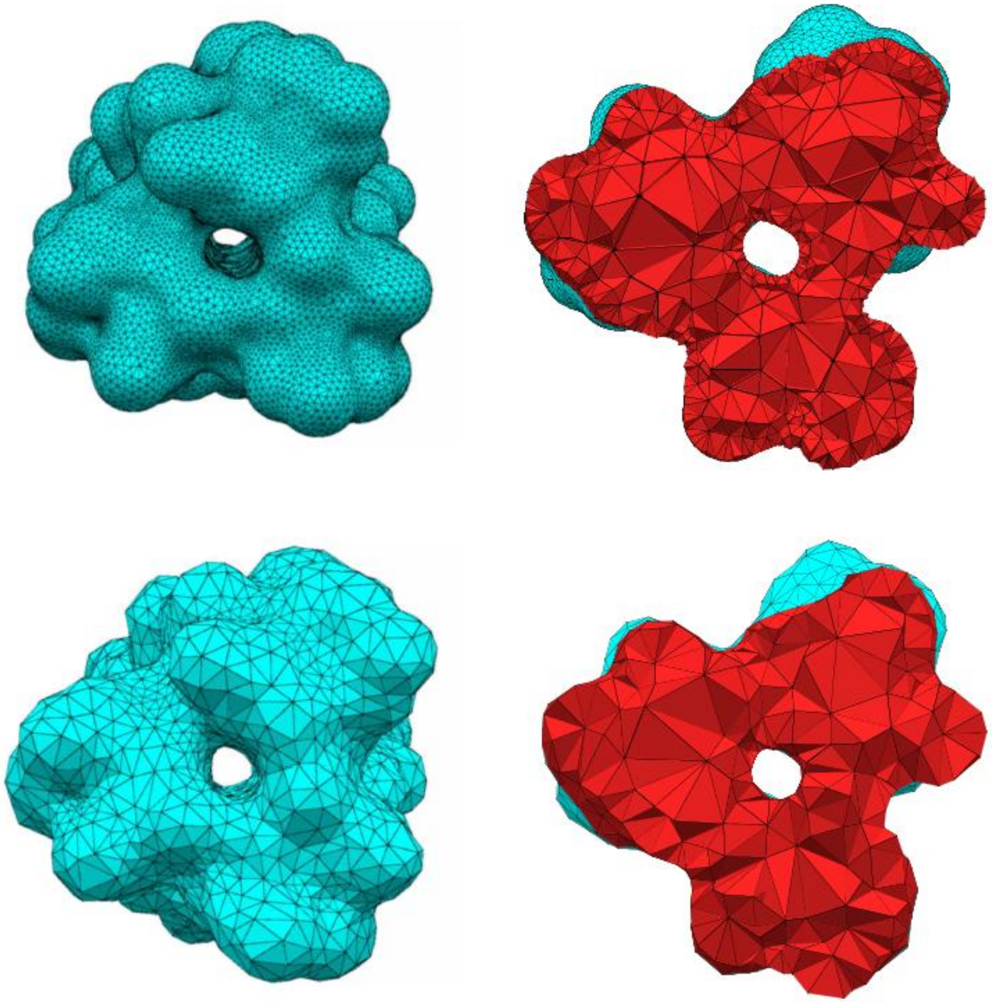
$$-\nabla\cdot(\epsilon(x)\nabla\phi(x)) + \bar{\kappa}^2(x)\sinh(\frac{e_c\phi(x)}{k_BT}) = 4\pi\,\Sigma_{i=1}^{N_m} q_i\delta(x - x_i)$$

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

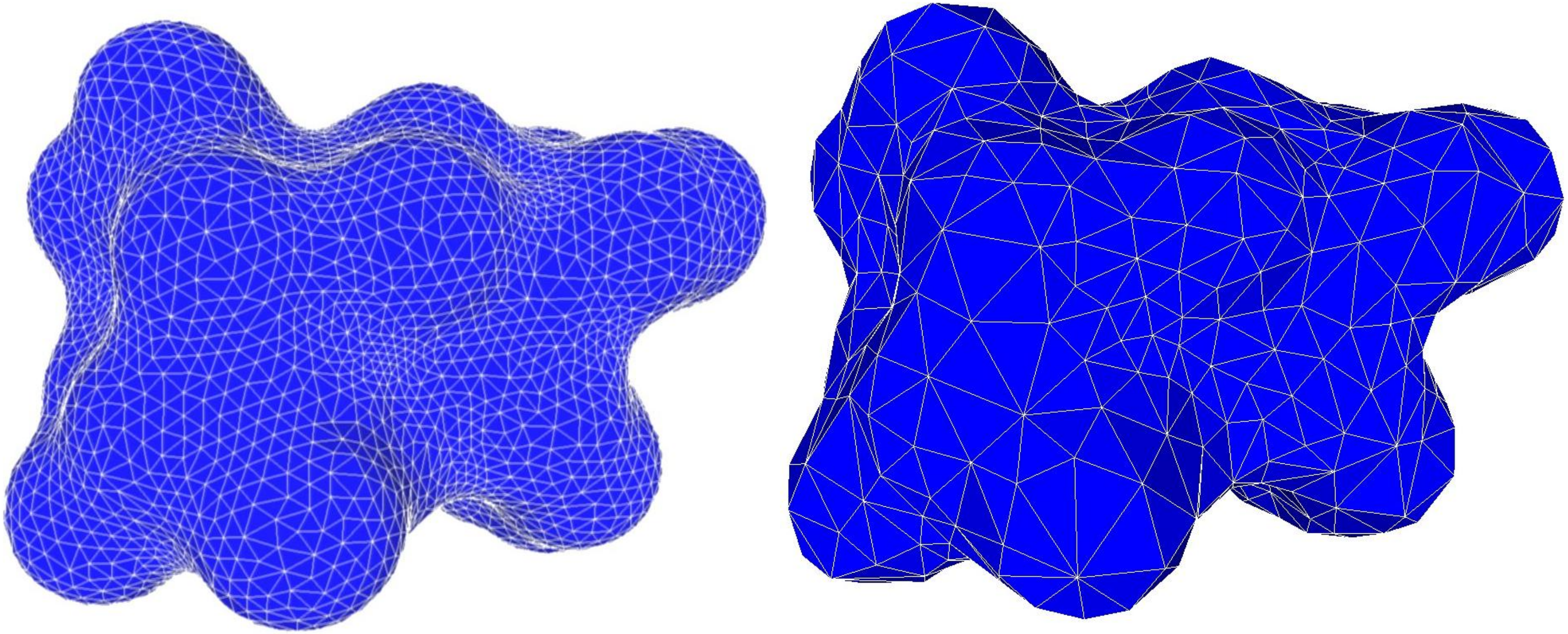
Mesh Coarsening

Hierarchical Mesh



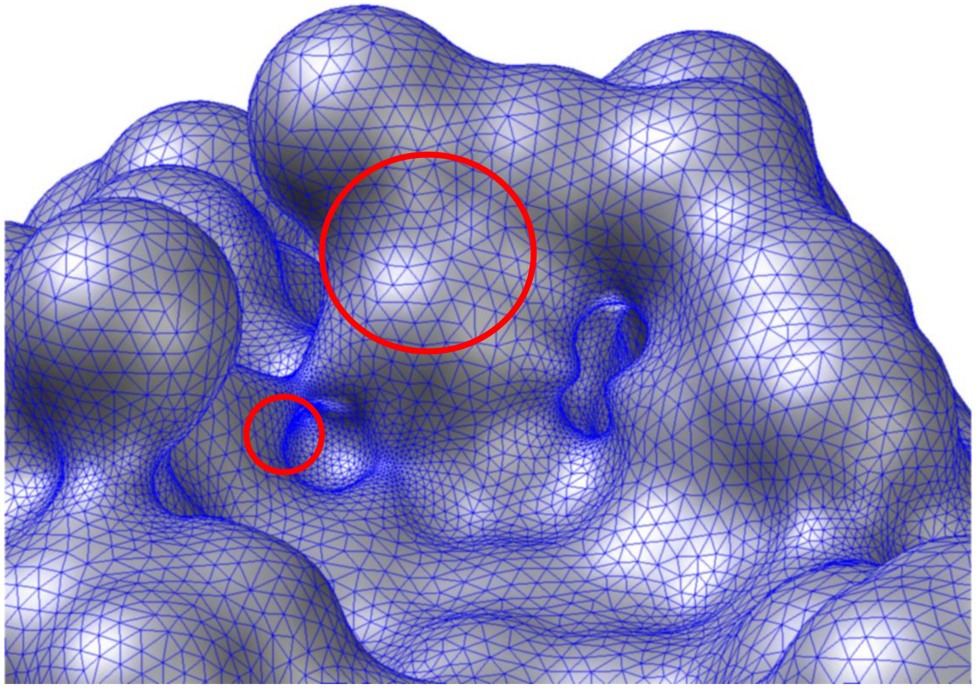
Mesh Coarsening

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



Adaptive Mesh

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

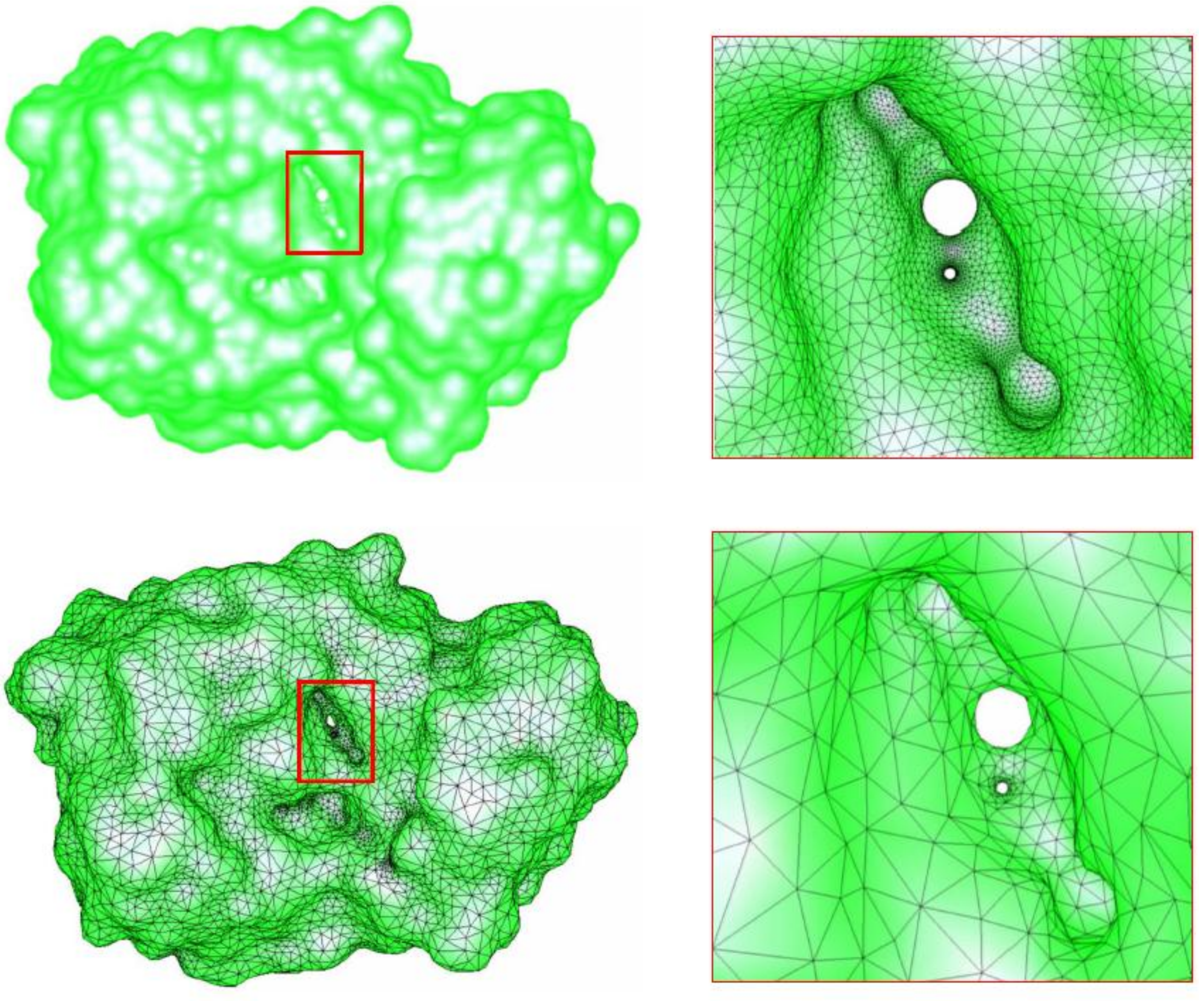


Algorithm

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

```
while eq is not empty do
    ab = deQueue(eq);
    edgeContraction(ab);
    Update fs;
    flipEdges(fs);
    Update eq and ts ;
    vertInsertion(ts);
    Update fs;
    flipEdges(fs);
end while
```

Results



Results

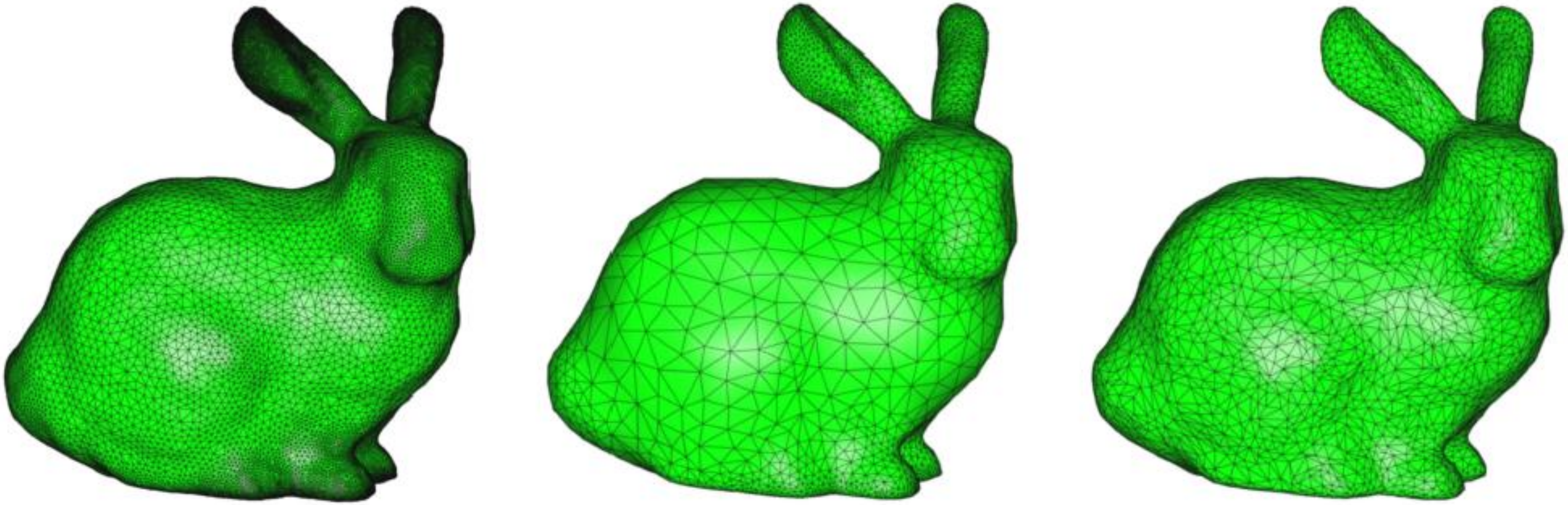


Fig. 8. *A comparison of our skin mesh coarsening algorithm with Qslim.*

Discussions

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

Questions