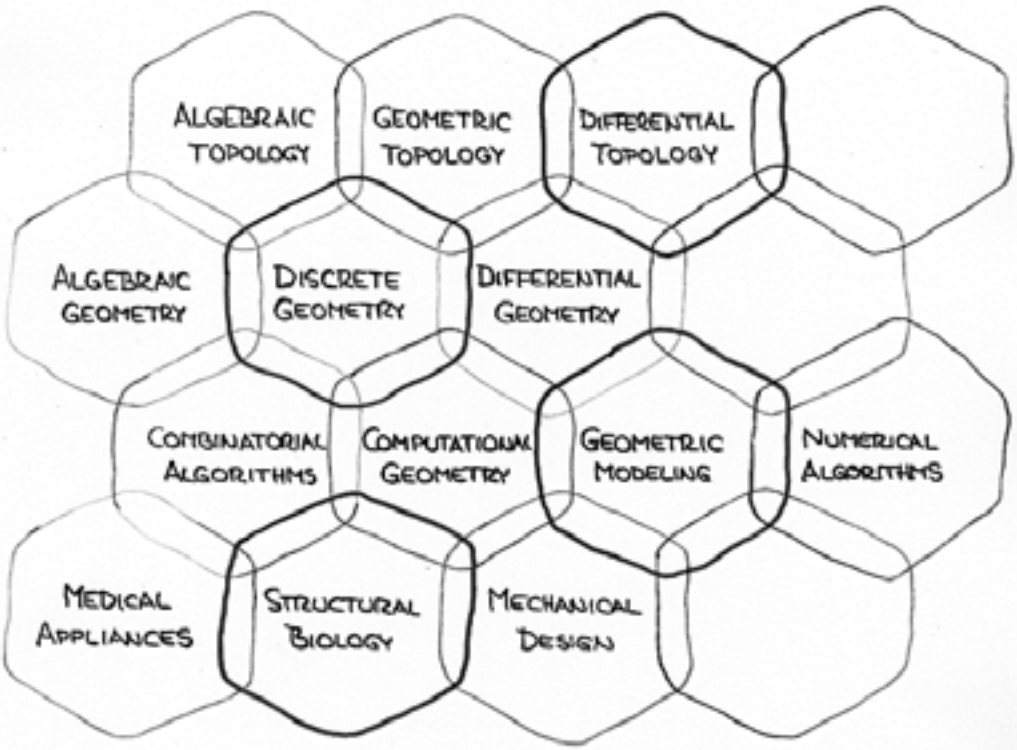
COMPUTATIONAL TOPOLOGY

APPLICATIONS-DRIVEN



HEARING-AIDS

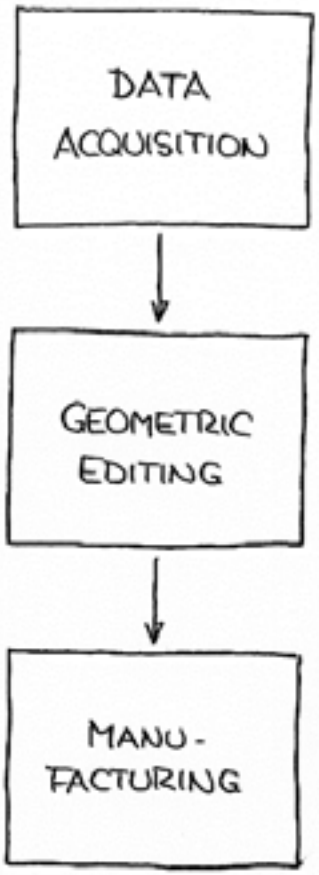
DRILLING + TRIMMING

ORTHODONTICS

SCANNING
SURFACE RECONSTRUCTION

FEATURE DETECTION
MOTION PLANNING

3D PRINTING



STRUCTURAL BIOLOGY

I MODELS

II CONNECTIVITY

III SIZE

IV SHAPE AND FIT

V METAMORPHOSIS

I MODELS

(a) VAN DER WAALS

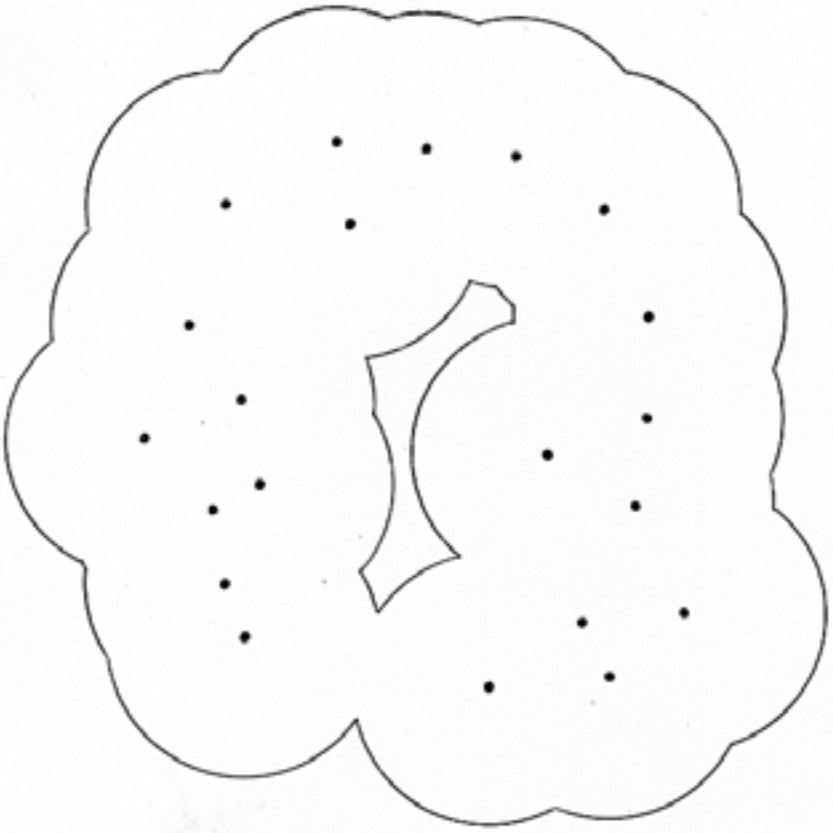
(b) SOLVENT ACCESSIBLE

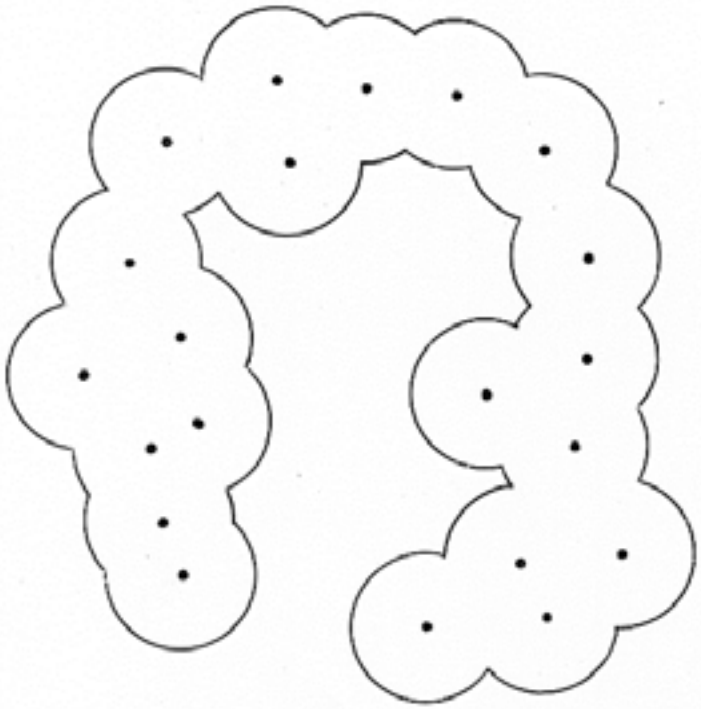
(c) MOLECULAR SURFACE

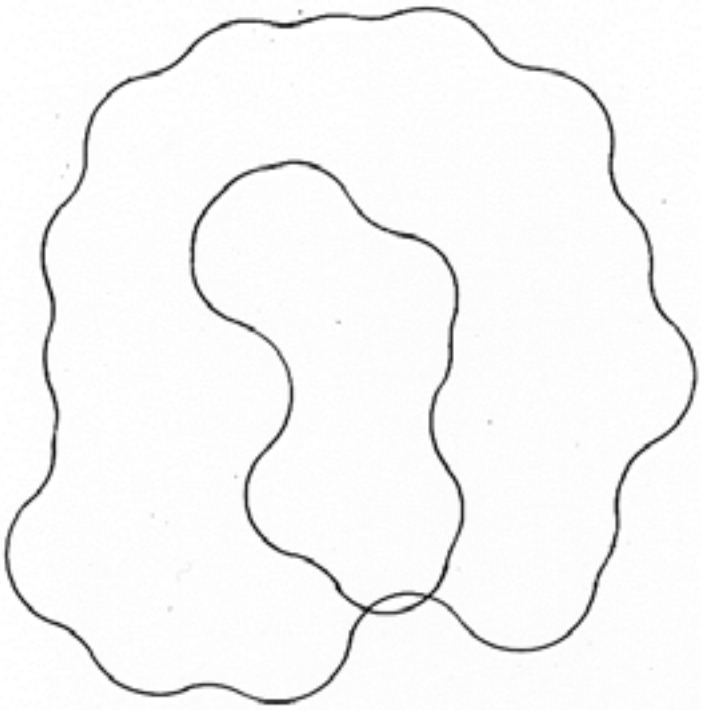
(d) VORONOI, DELAUNAY

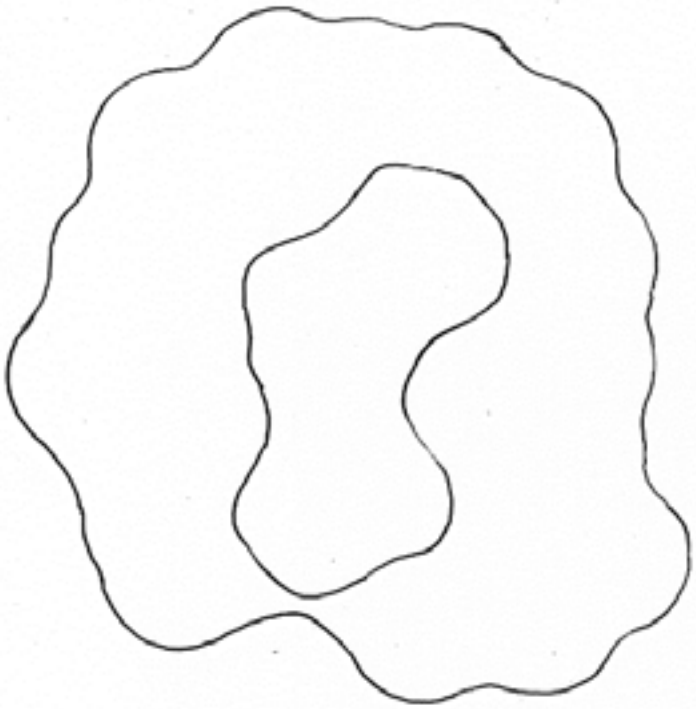
(e) ALPHA SHAPE

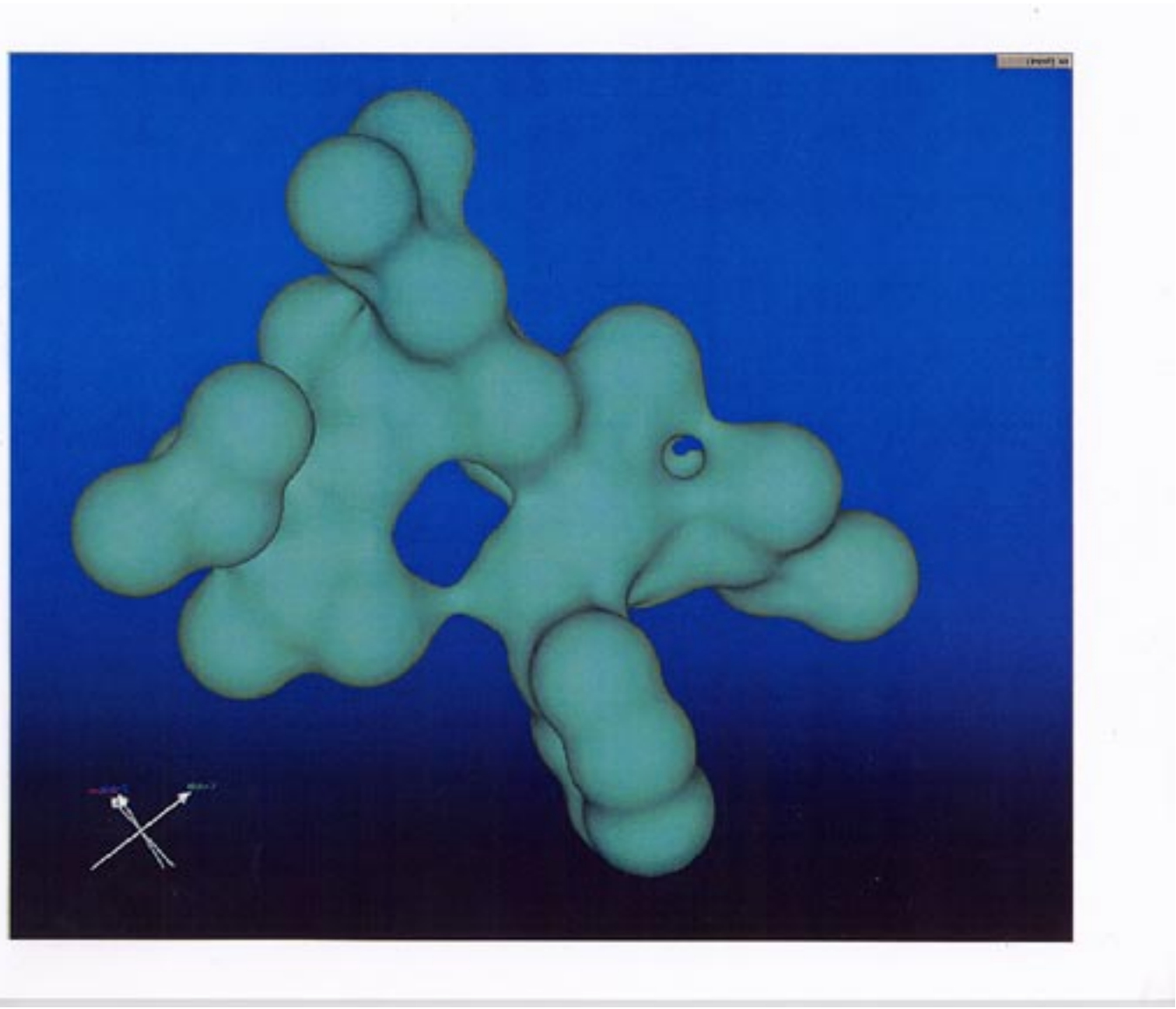
(f) SKIN SURFACE

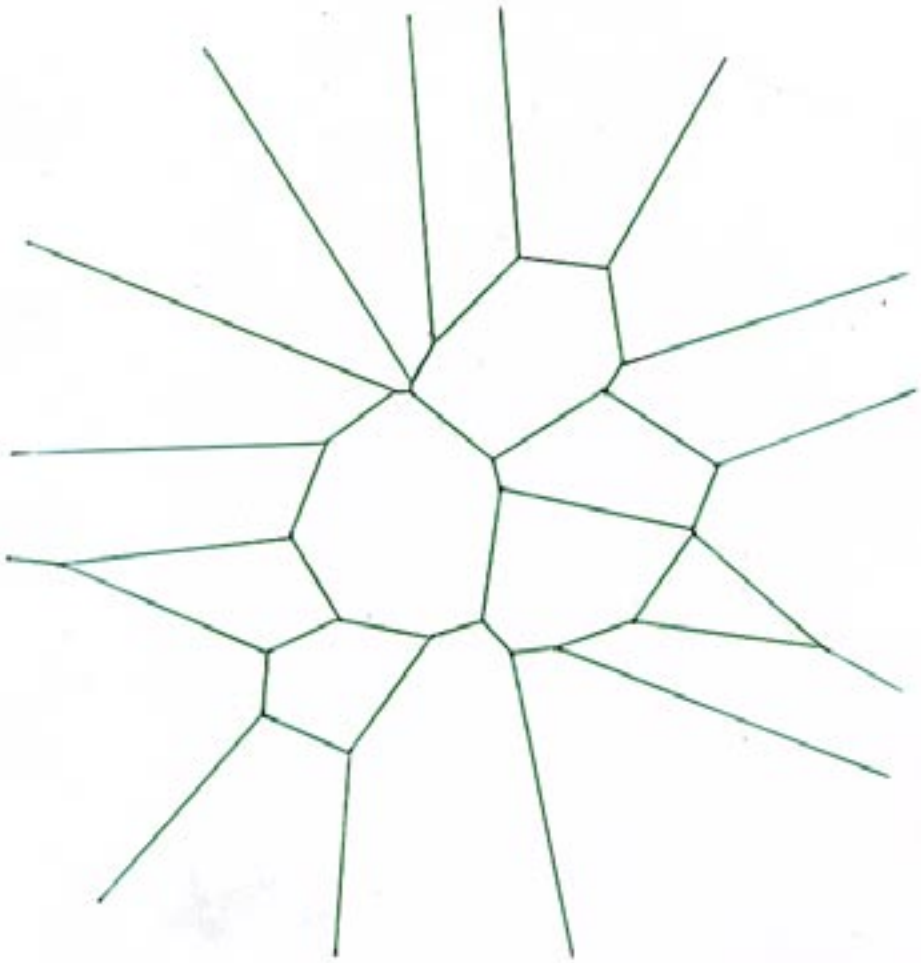


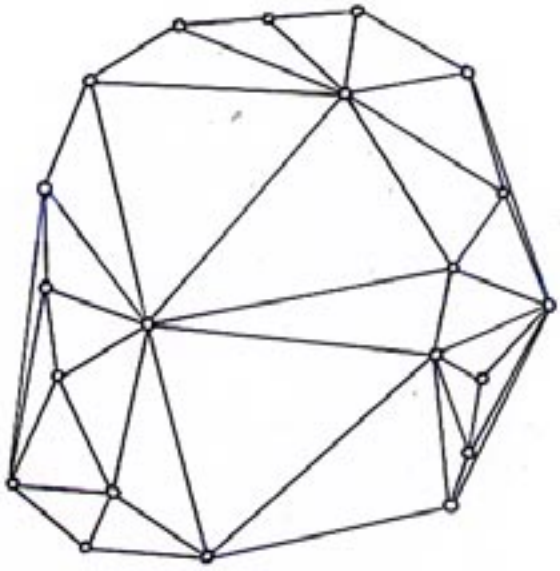


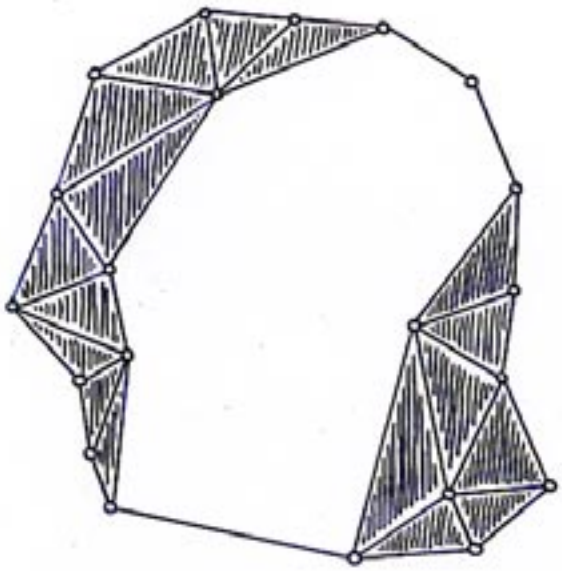


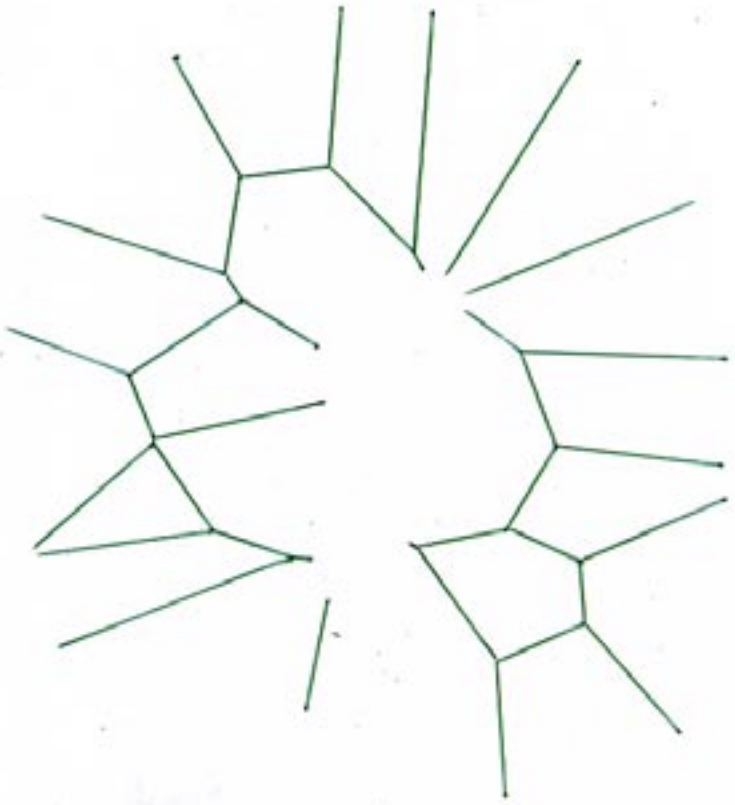


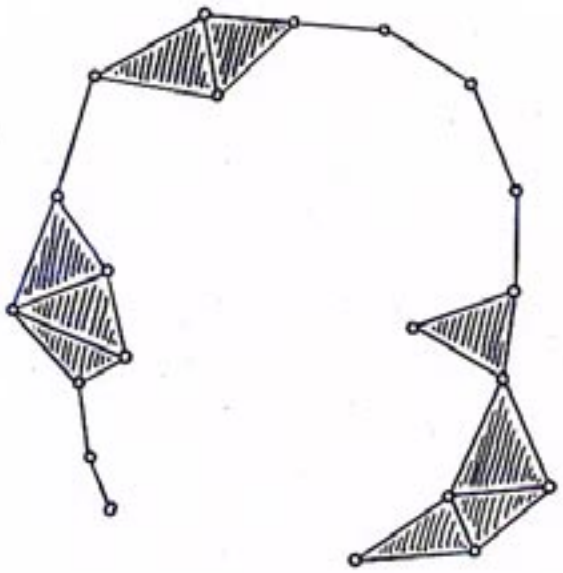












II. Connectivity

(a) Homotopy Equivalence:

$\cup B \simeq |K|$.

(b) Betti Number Algorithm.

(c) Pockets.

(d) Persistence

$$\underbrace{\sigma_0, \sigma_1, \dots, \sigma_{j-1}, \sigma_j}_{= K = K_j}, \underbrace{\sigma_{j+1}, \dots, \sigma_n}_{= D - K}$$

FILTER: EVERY PREFIX IS A COMPLEX

$$K_0, K_1, \dots, K_{j-1}, K_j, K_{j+1}, \dots, K_n$$

FILTRATION $(K_i = \{\sigma_0, \sigma_1, \dots, \sigma_i\})$

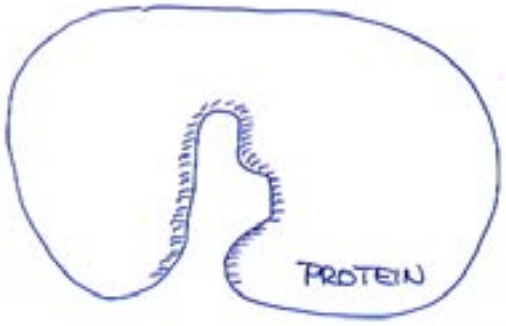
ALGORITHM FOR BETTI NUMBERS

```
integer^3 BETTI (K_j):
    β_0 = β_1 = β_2 = 0;
    for i = 0 to j do
        k = dim σ_i ;
        if σ_i belongs to k-cycle in K_i
            then β_k ++
            else β_{k-1} --
        endif
    endfor ;
    return (β_0, β_1, β_2).
```

TIME = $O(n \cdot \alpha(n))$.

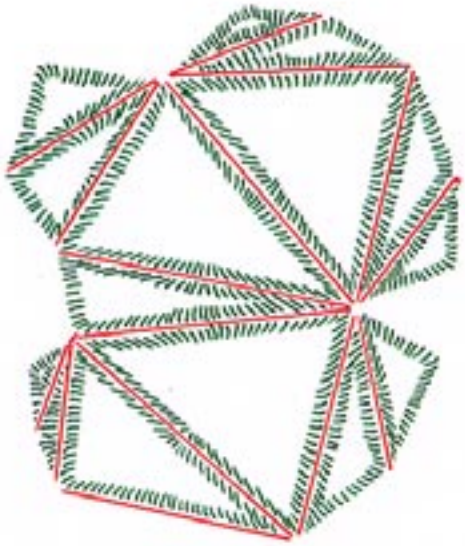
POCKETS (CAVITIES)

RECOGNITION BY COMPLEMENTARITY
(Lock and key mechanism)



Shape and energy complementarity

A pocket is a connected region outside U.A; that becomes a void before it disappears.



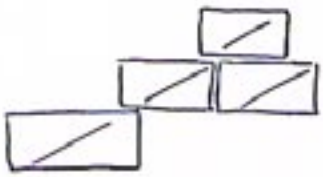
data: cdk2.xz
points: 2364
pocket no. 183 (8 months)
marked rank: 82108

III. Size

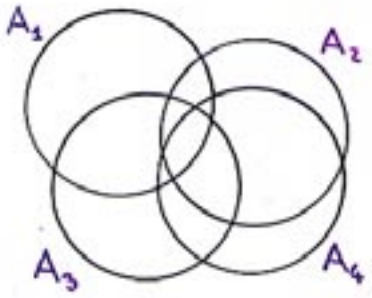
(a) PIE Formula

(b) Void Formula

(c) Area Derivative



THM. $\text{area } \bigcup_i A_i = \sum_{\sigma \in K} (-1)^{\dim \sigma} \cdot \text{area } \bigcap \sigma$



$$\begin{aligned}\text{area } \cup_i A_i = {} & A_1 + A_2 + A_3 + A_4 \\ & - A_{12} - A_{13} - A_{14} - A_{23} - A_{24} - A_{34} \\ & + A_{123} + A_{124} + A_{134} + A_{234} \\ & - A_{1234}.\end{aligned}$$

DEPTH - 2 FORMULA (AND VOIDS)

THM. $\text{area} \bigcup_i A_i = \sum_{\sigma^2 \in K} \text{area}\, \sigma^2 + \sum_{\sigma \le \tau} (-1)^{\dim \sigma} \cdot \varphi_{\sigma,\tau} \cdot \text{area} \cap \sigma.$

$\sigma \in K$, $\tau \in \mathcal{D}\text{-}K$

$\varphi_{\sigma,\tau}$: angle at σ inside τ

Area Derivative :

The derivative of the area of $\cup B$ is

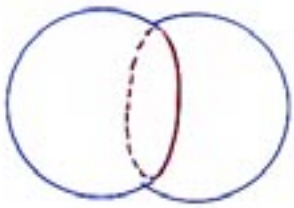
$$DA_B : \mathbb{R}^{3n} \to \mathbb{R}$$

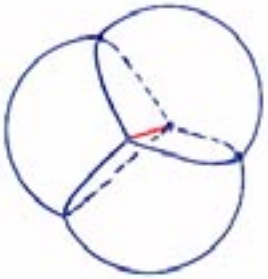
defined by $DA_B(t) = \langle a, t \rangle$ with

$$\begin{bmatrix} a_{3i+1} \\ a_{3i+2} \\ a_{3i+3} \end{bmatrix} = \sum_j \left(\sigma_{ij} a_{ij} + \sum_k \beta_{ijk} a_{ijk} \right),$$

$$a_{ij} = \pi(\rho_i + \rho_j)\left[1 - \frac{(\rho_i - \rho_j)^2}{\zeta_{ij}^2}\right] u_{ij}$$

$$a_{ijk} = 2\rho_{ijk} \frac{\rho_i - \rho_j}{\zeta_{ij}} u_{ijk}$$



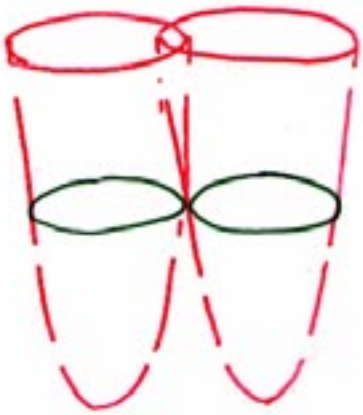


IV Shape & Fit

(a) Vector Space

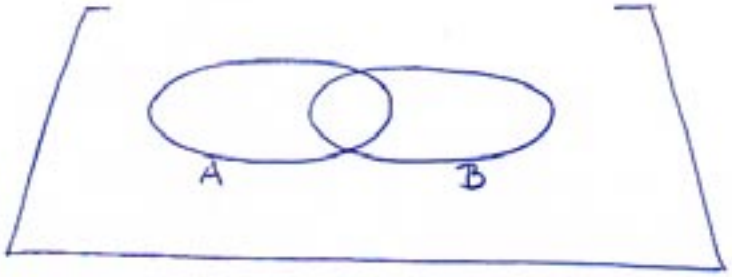
(b) Body & Skin

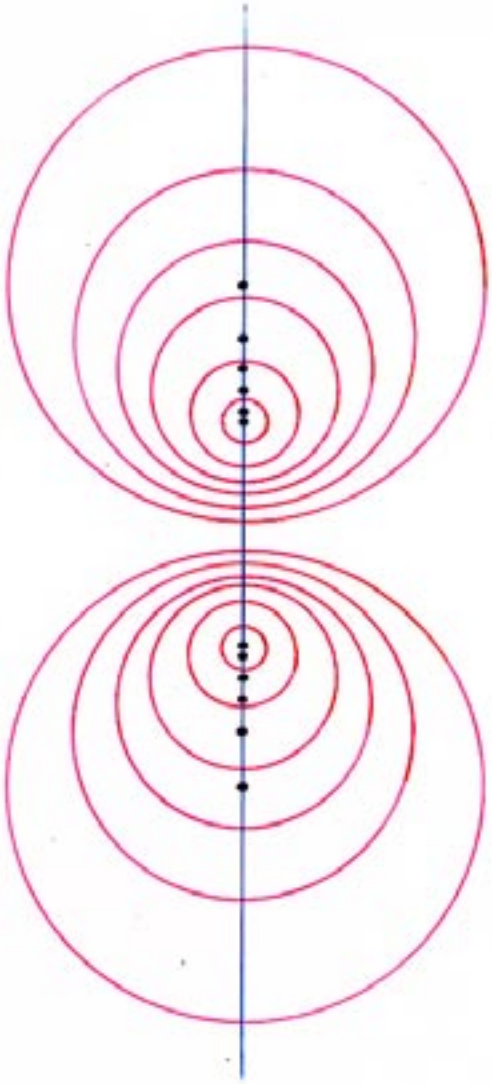
(c) Symmetry

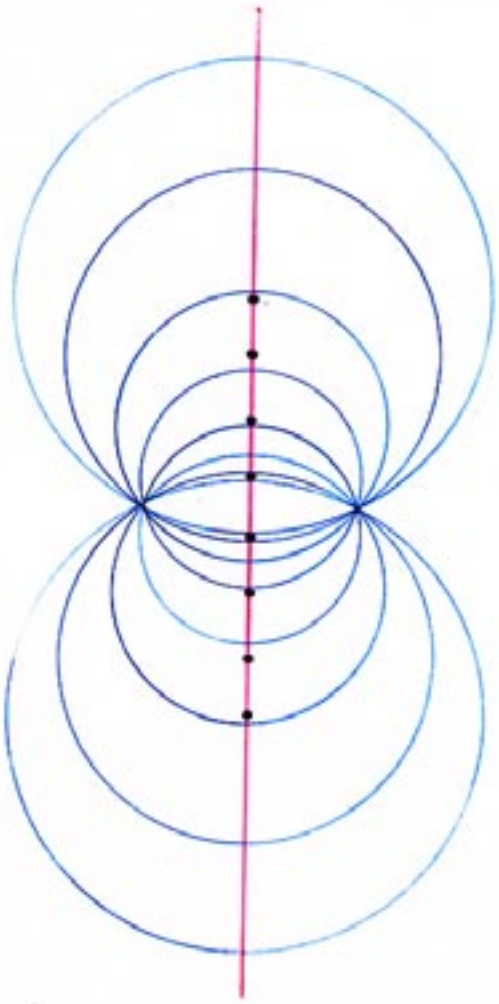


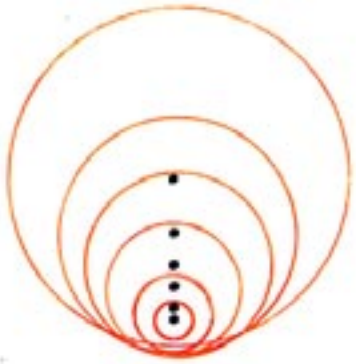
$$\delta(x) = \|x - p\|_5 - \varepsilon_5 \qquad \beta = \delta_{-2}(0)$$
$$\ell(x) = \|x - q\|_5 - \lambda_5 \qquad V = \ell_{-2}(0)$$

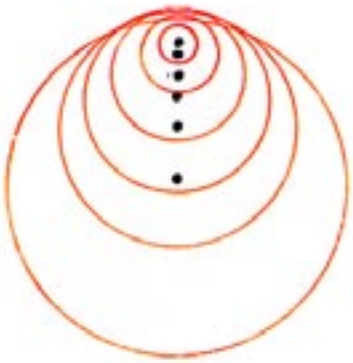
Vector Space of Circles

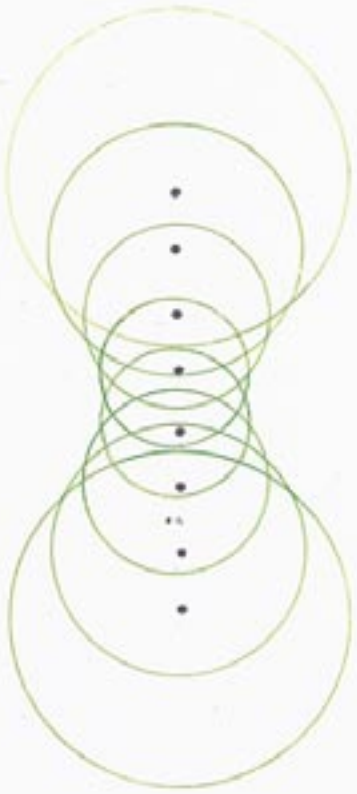


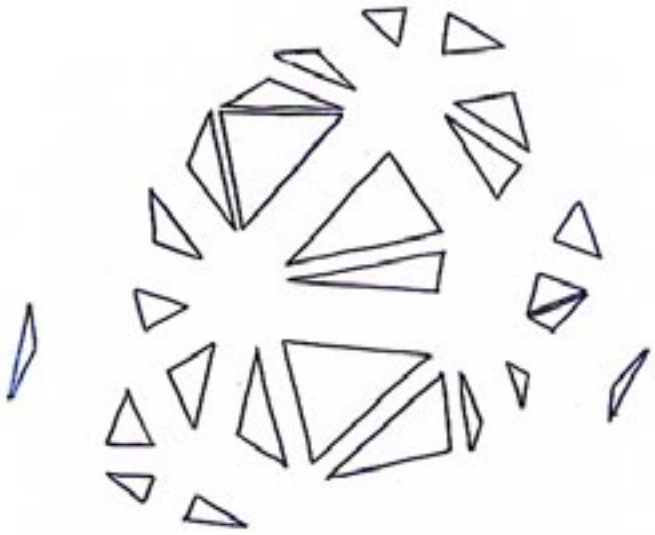


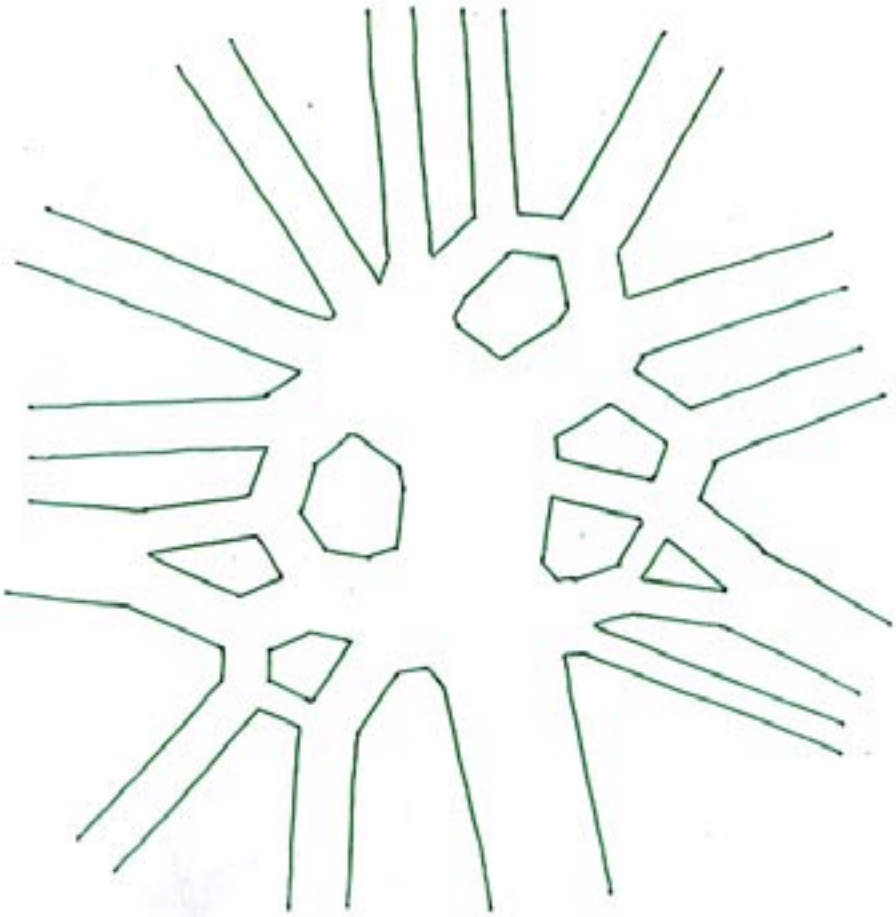


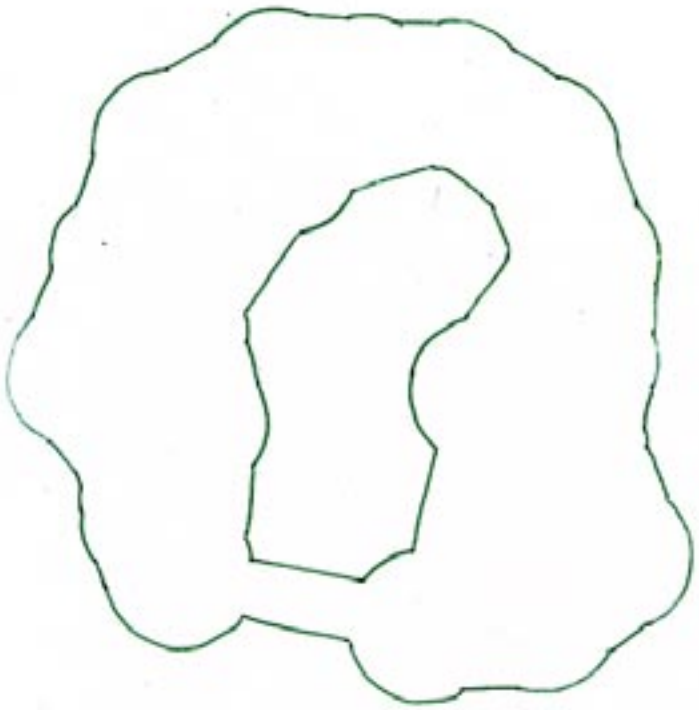


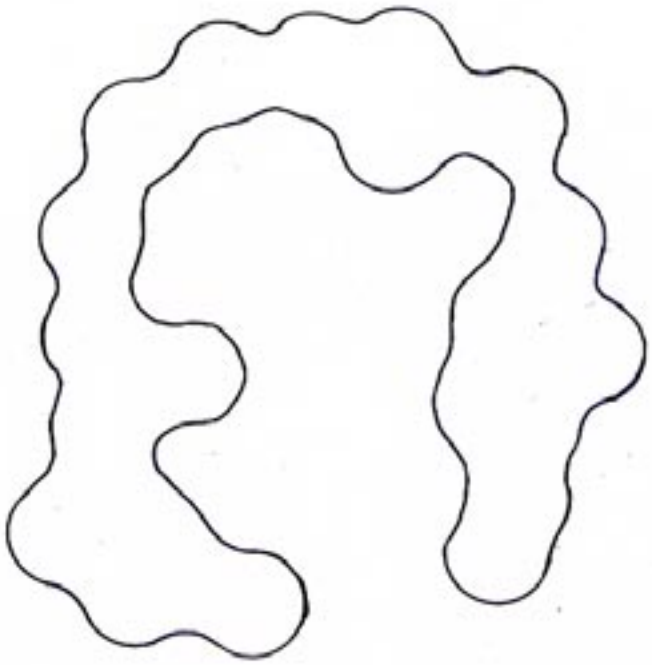


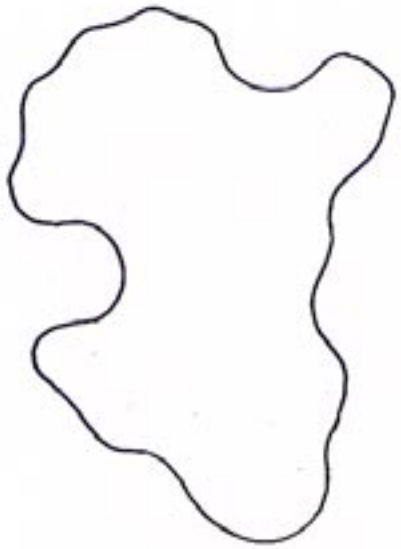


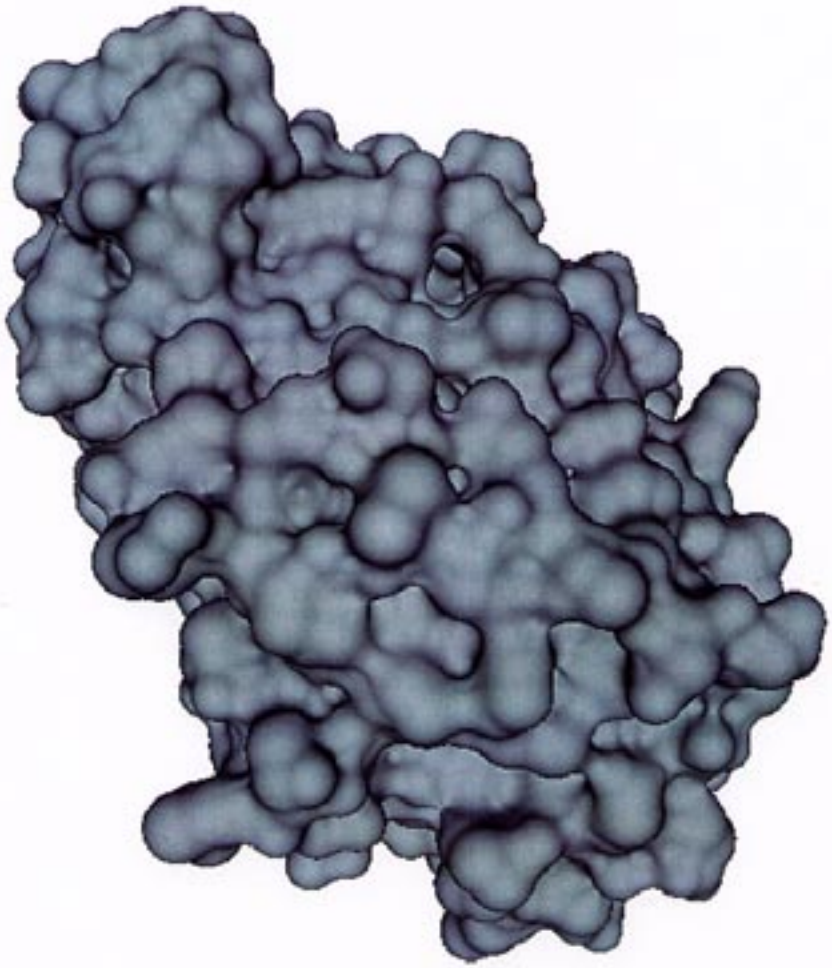


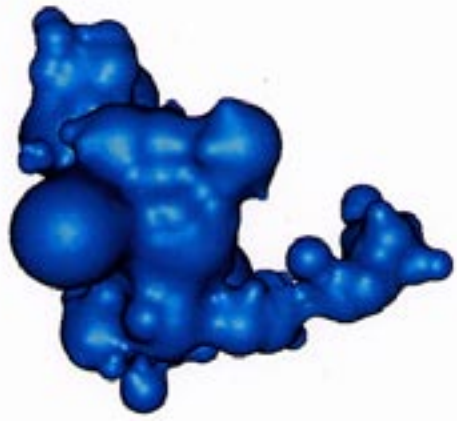


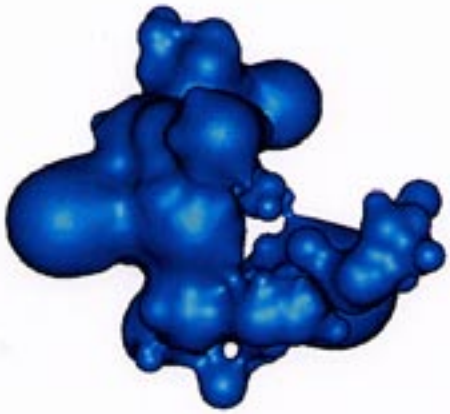












V. METAMORPHOSIS

(a) MIXED VOLUME

(b) DYNAMIC MESHING

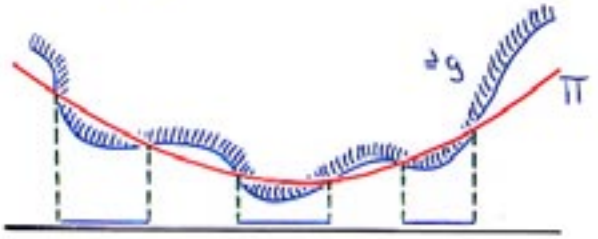
(c) TOPOLOGY OPTIMIZATION

GEOMETRIC CONSTRUCTION

$$\text{shape}^d = \text{proj}\left[\text{conv}^{d+1} \cap \text{bd conv}^{d+1}\right].$$

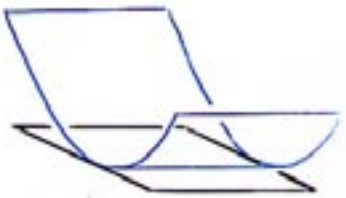
above graph of $g : \mathbb{R}^d \to \mathbb{R}$

graph of $\Pi : \mathbb{R}^d \to \mathbb{R}$ defined by $\Pi(x) = \|x\|^2$

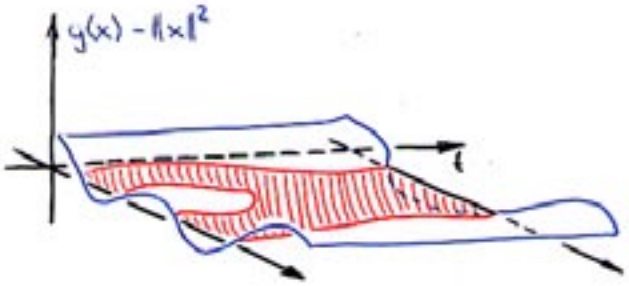


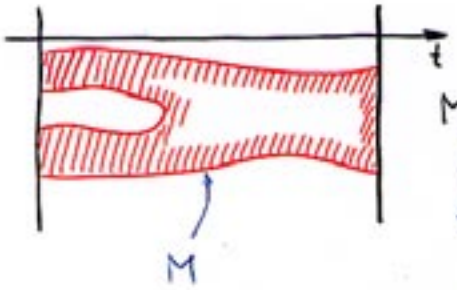
MAIN STEPS.

1. $X_0, X_1 \subseteq \mathbb{R}^d$ represented by $g_0, g_1 : \mathbb{R}^d \to \mathbb{R}$
2. deformation through mixed volume and sweep in $\mathbb{R}^{d+1} \times [0, 1]$.



Morse Theory Interpretation





Morse function

$f : M \to \mathbb{R}$

$f(x) = t$

shapes are $f^{-1}(t)$.

topology changes at critical points.

TOPOLOGY OPTIMIZATION

3D EXTRUSION BRIDGE DIE
INJECTION MOLD
MEMS
} DESIGN

ADAPTATION

TO SHAPE

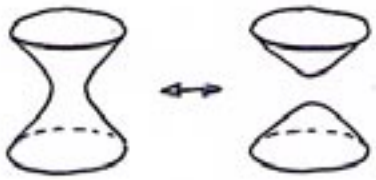
e.g. move vertices along gradient

TO CURVATURE

$$\text{mesh density} \sim \frac{1}{\text{max curvature function}}$$

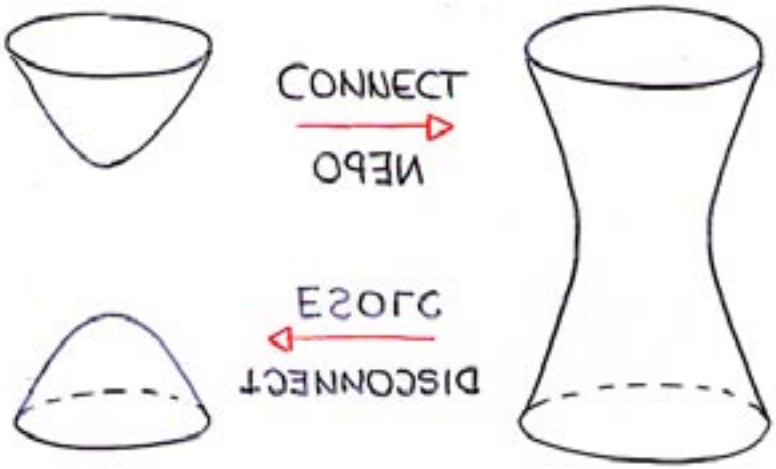
e.g. maintained through point insertions and edge contractions

TO TOPOLOGY



TOPOLOGY

(HANDLES & TUNNELS)



TOPOLOGY

(COMPONENTS & VOIDS)

CREATE

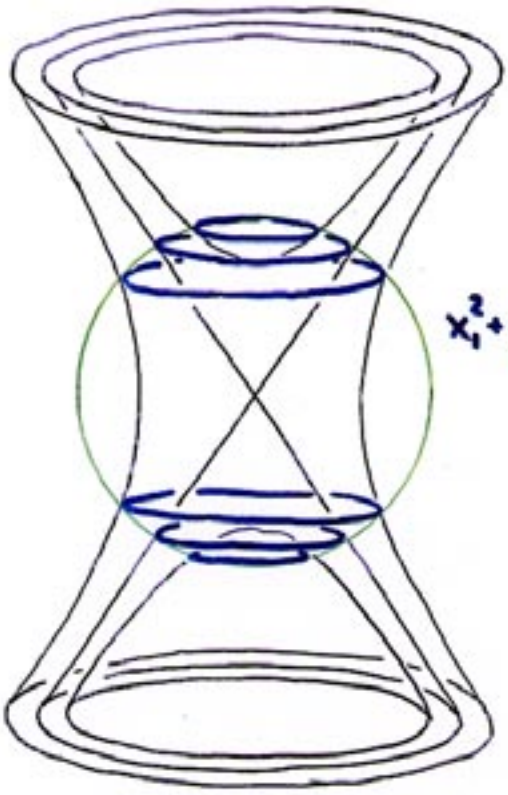
HOLLOW

$\emptyset$

FILL

DESTROY

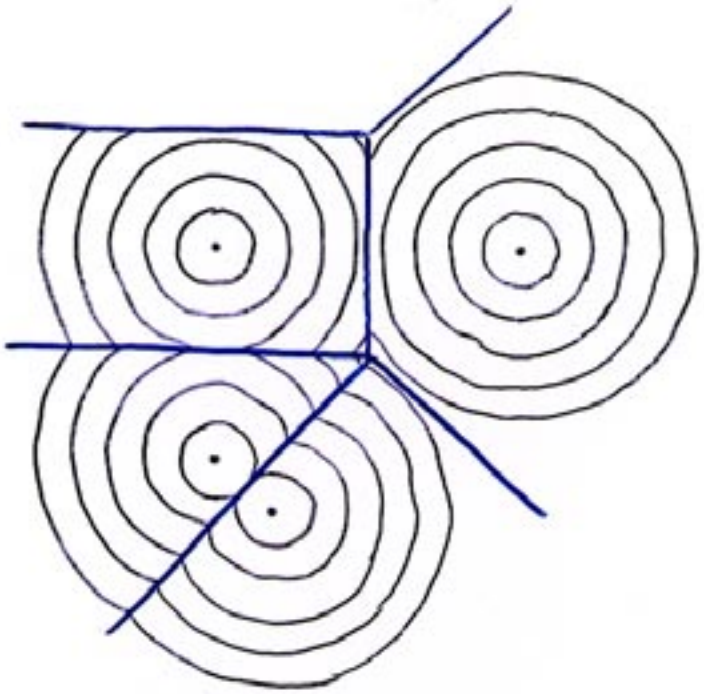
ISO CURVATURE



$x_1^2 + x_2^2 + x_3^2 = \frac{1}{K}$

$x_1^2 + x_2^2 - x_3^2 = \text{const.}$

CURVATURE VARIATION



$$\left|\frac{1}{\kappa(x)} - \frac{1}{\kappa(y)}\right| \leq \|x-y\|$$

III.3 DENSITY