Alpha Shapes Extended

Singapore 2017

Herbert Edelsbrunner
IST Austria

I BioGeometry

II Wrap

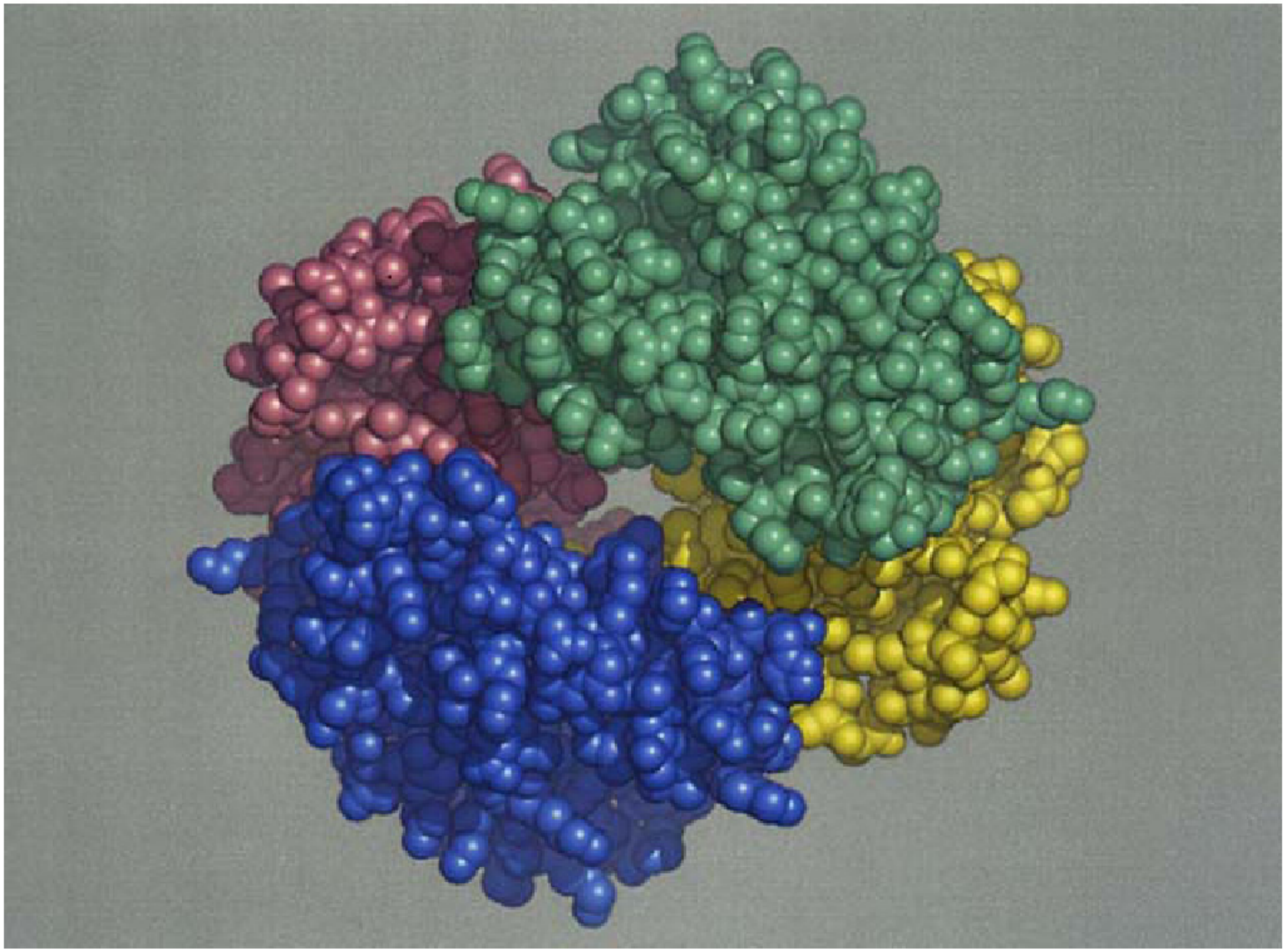
III Persistence

IV Expectation

From Proteins to Simplicial Complexes

Hemoglobin

Oxygen transport



From Proteins to Simplicial Complexes

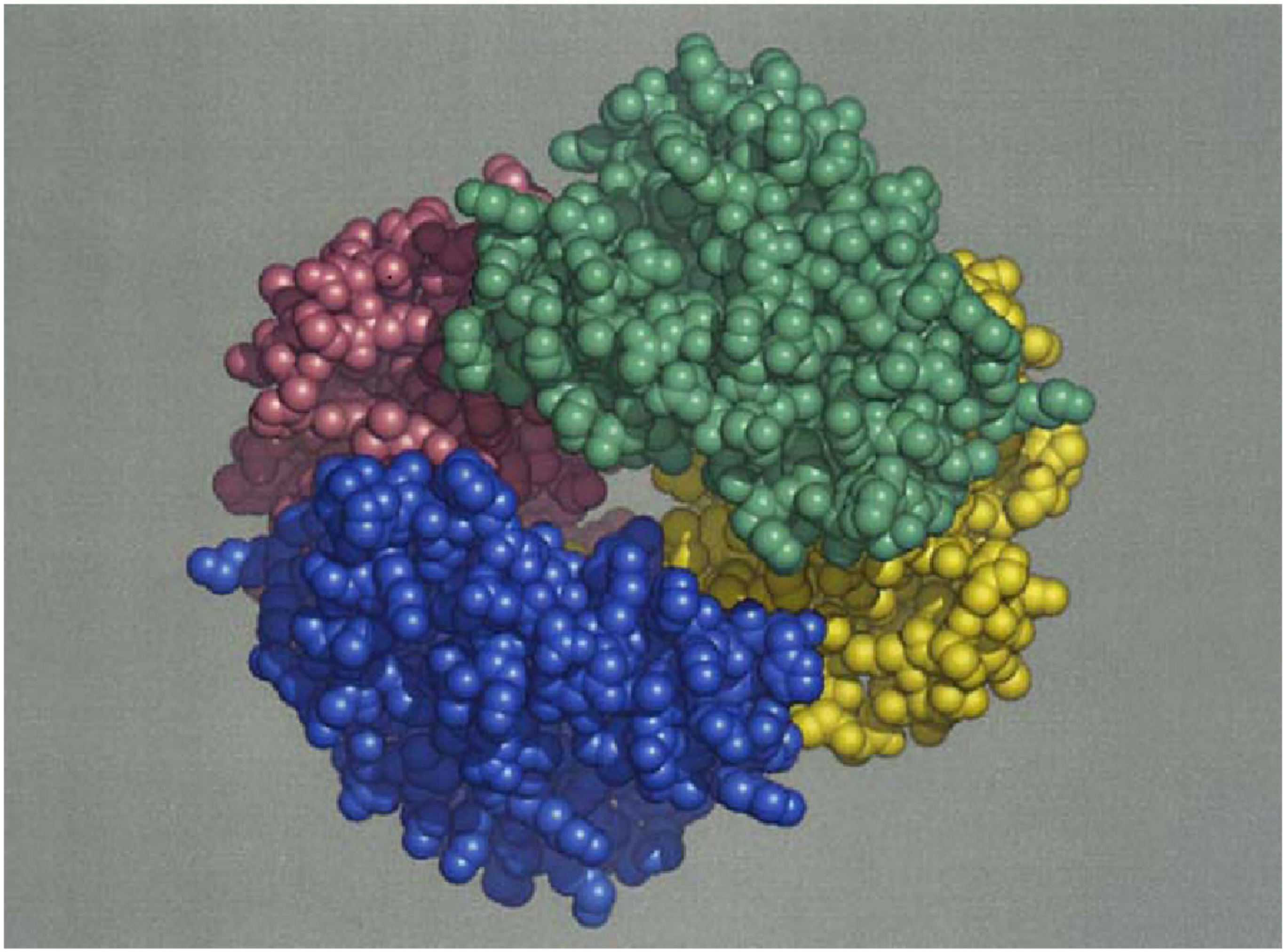
Hemoglobin

Oxygen transport

protein = $\bigcup$ balls in $\mathbb{R}^3$

Voronoi $\downarrow$ + nerve

α - complex



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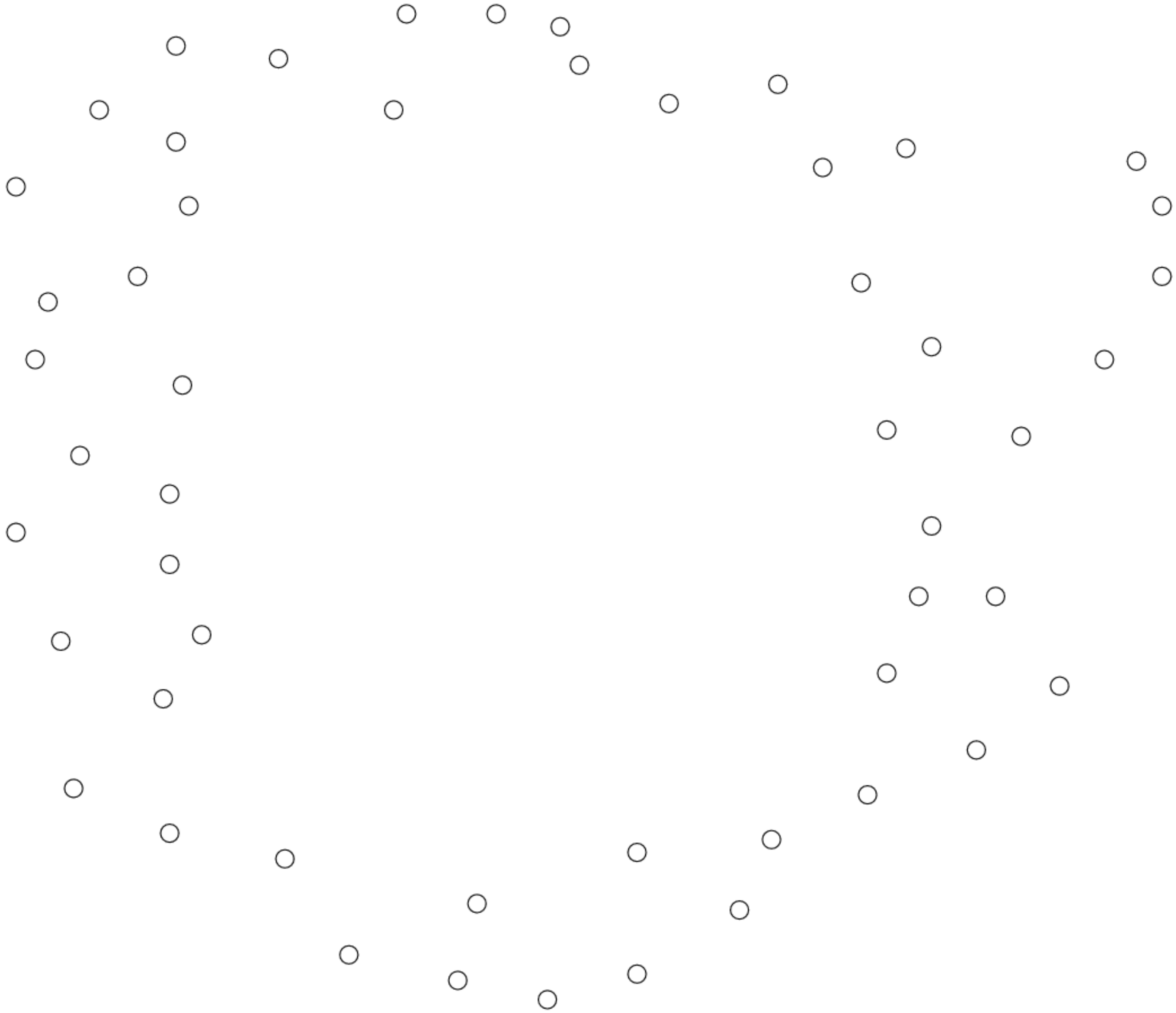

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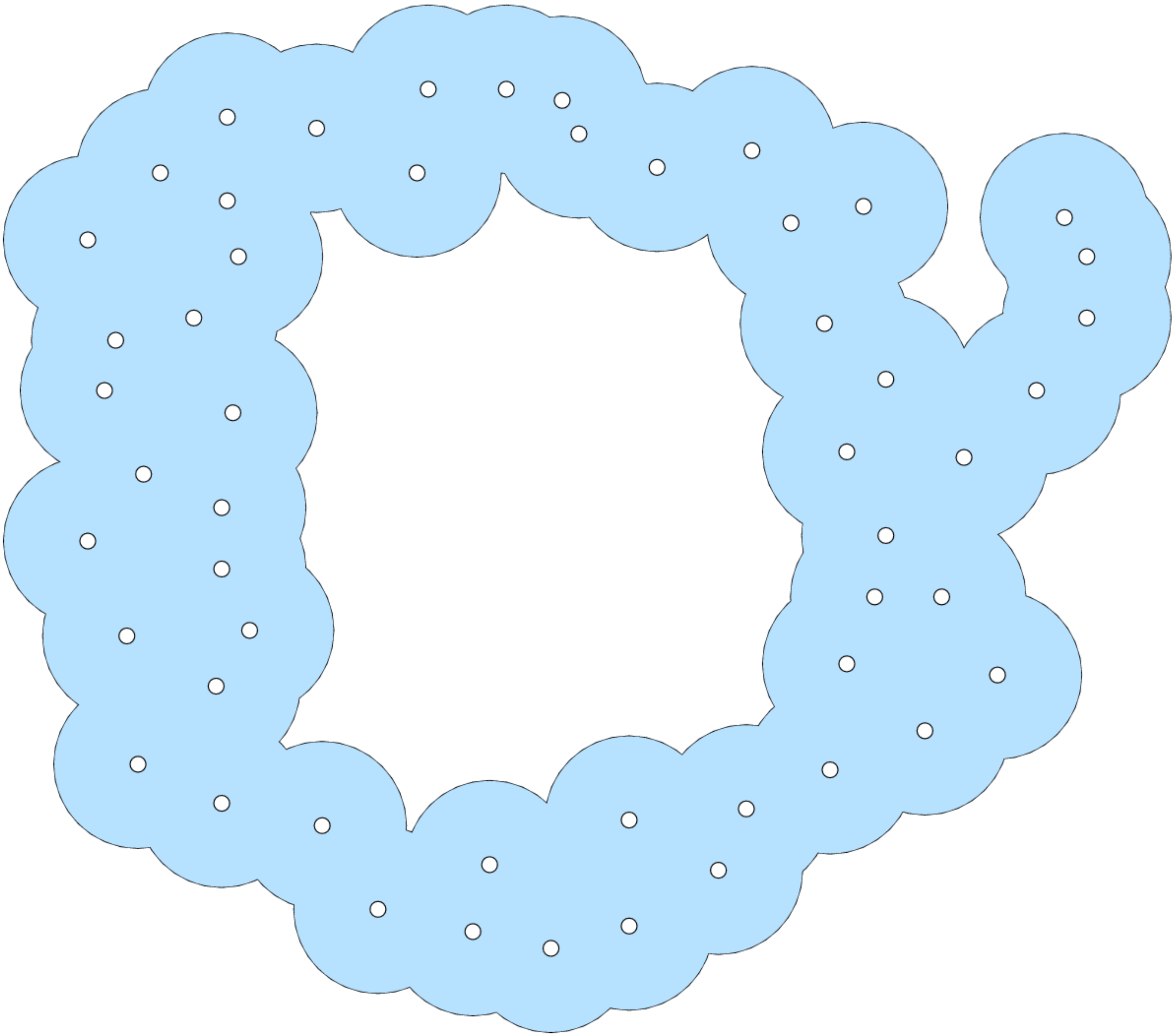

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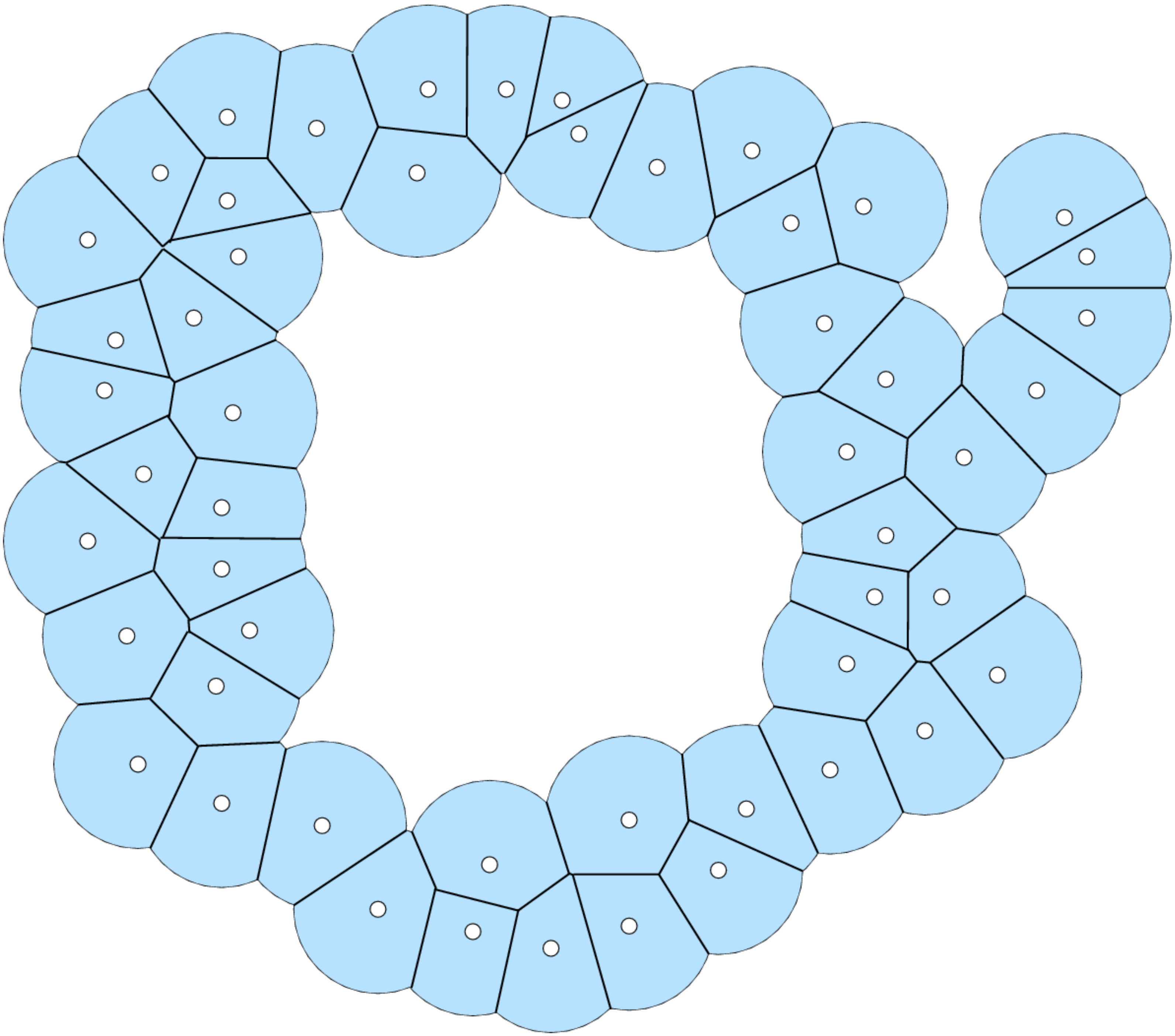
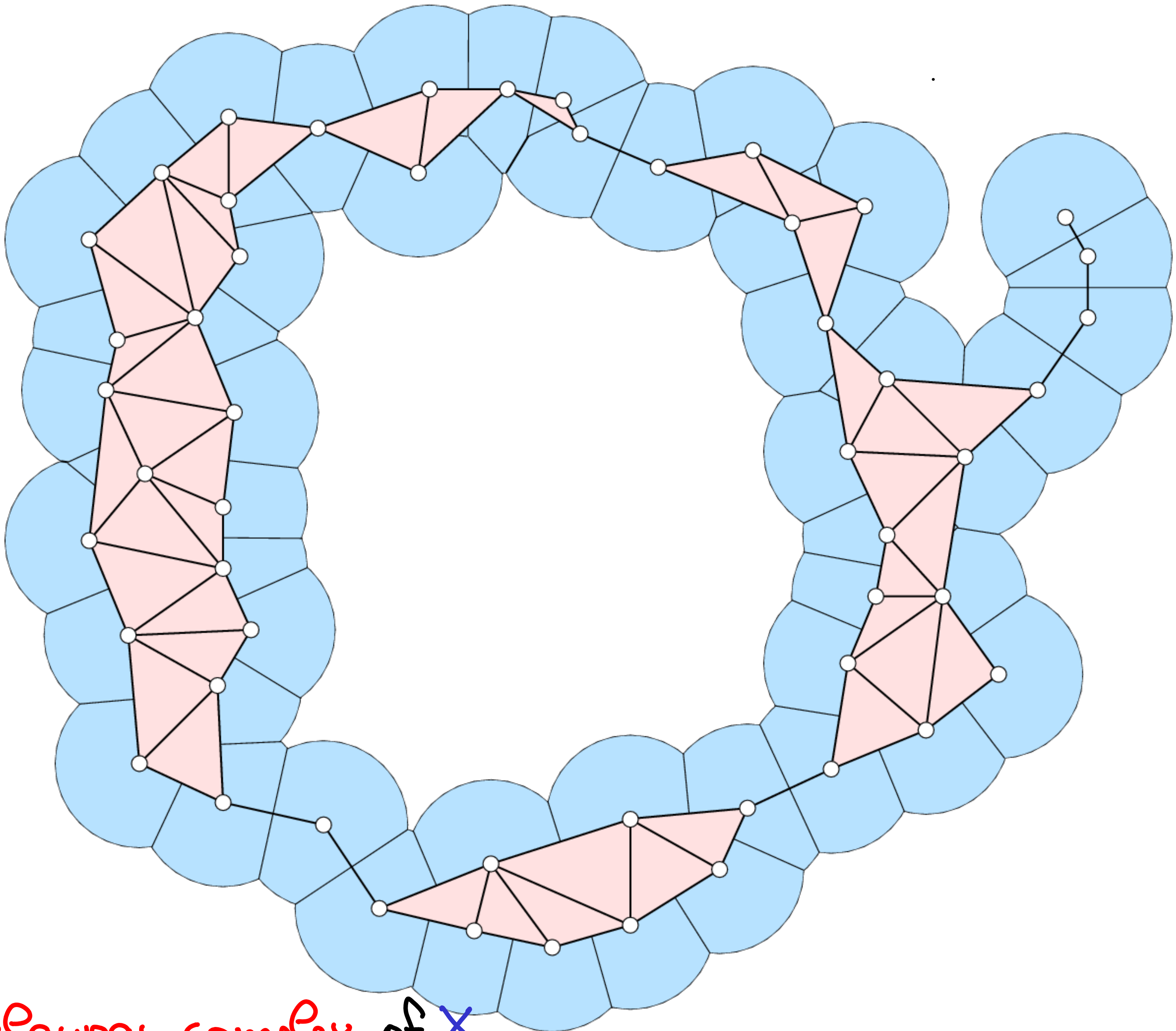


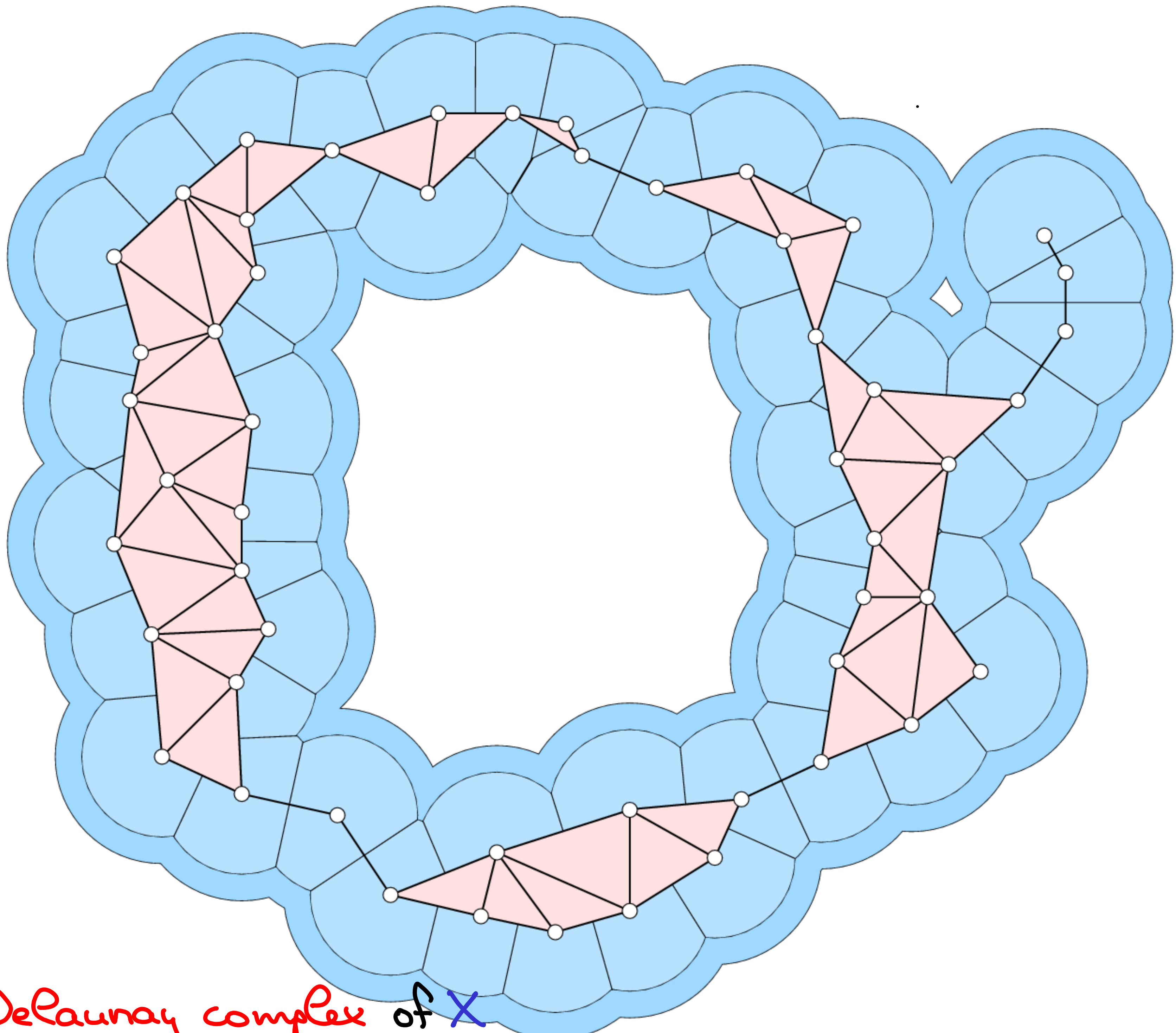
Voronoi domains $V(x)$

From Proteins to Simplicial Complexes



Delaunay complex of X for radius r is $D_r(X) = \{ P \subseteq X \mid \bigcap_{x \in P} [B_r(x) \cap V(x)] \neq \emptyset \}$.

From Proteins to Simplicial Complexes



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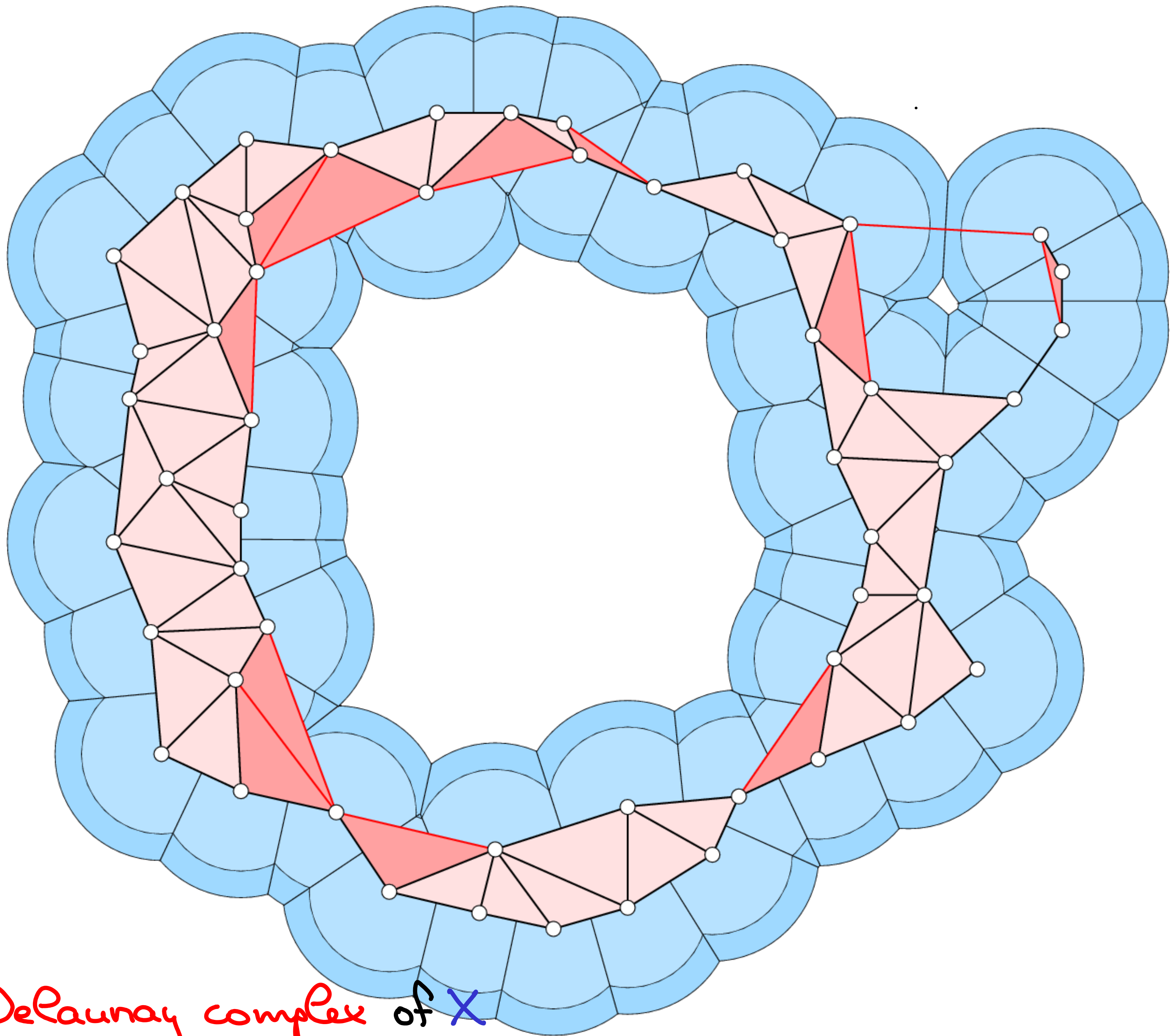

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Theorem:

$$\mathrm{Vol}(\cup B) = \sum_{Q \in D_r(X)} (-1)^{\dim Q} \, \mathrm{Vol}(\cap Q).$$

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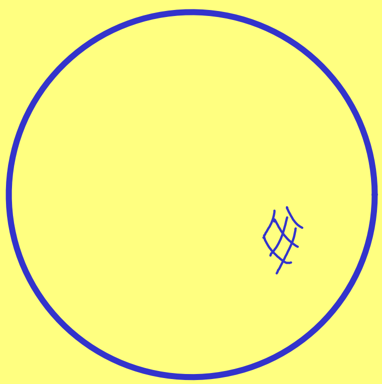

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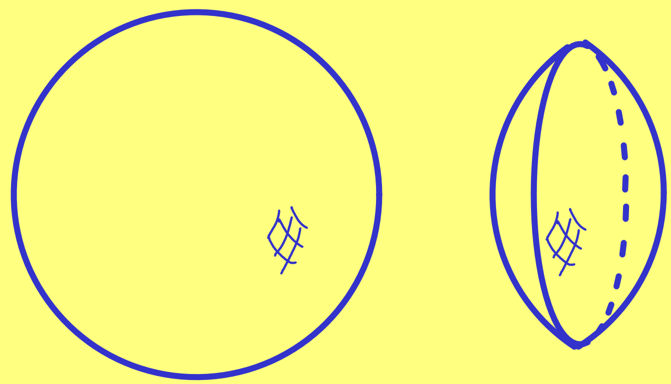

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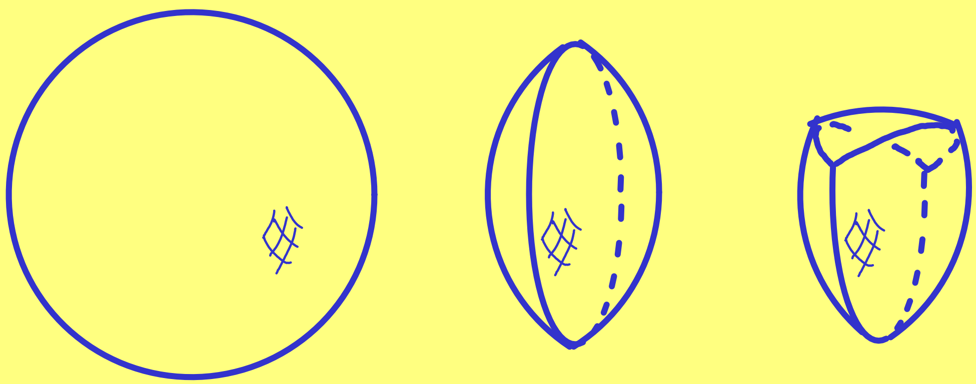

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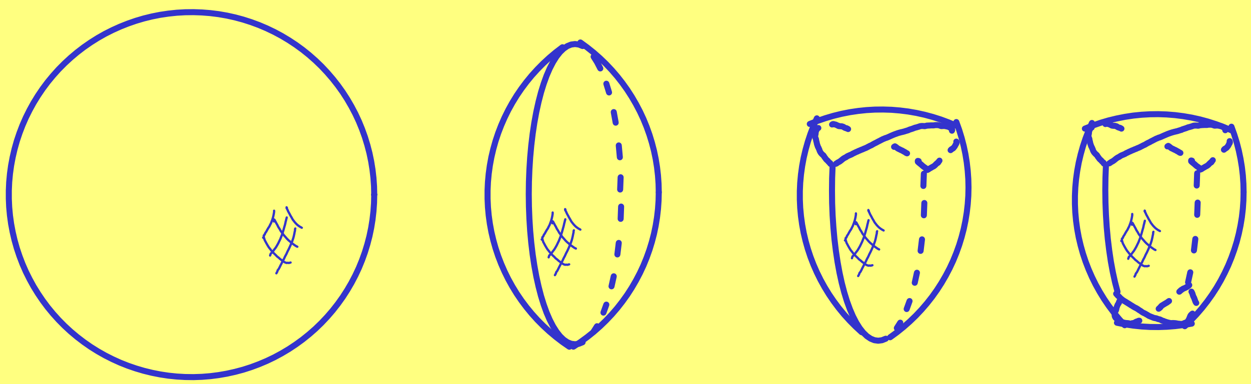

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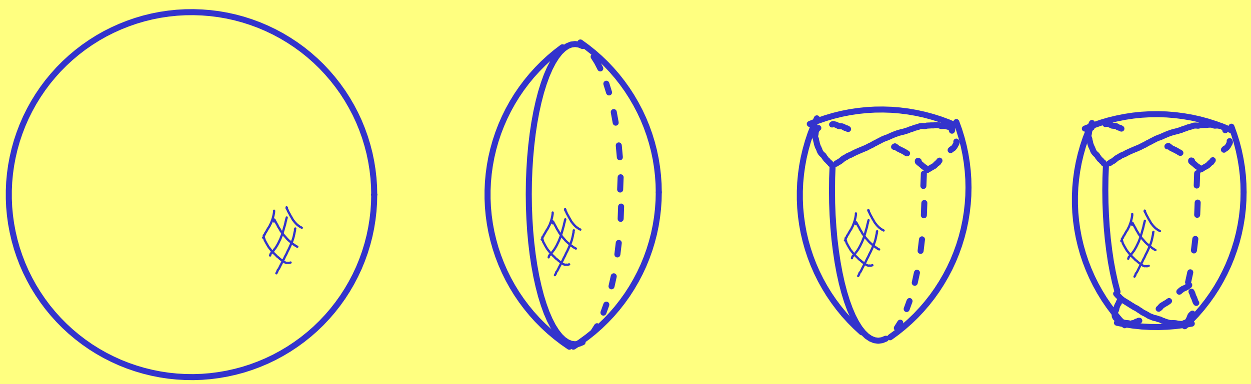

Extends to voids, pockets; area,

area derivative, volume derivative

Nerve Theorem

[Leray 1946]

NERVE THEOREM

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$$D_r(X) = \text{Nerve}\{B_r(x) \cap V(x) \mid x \in X\}.$$

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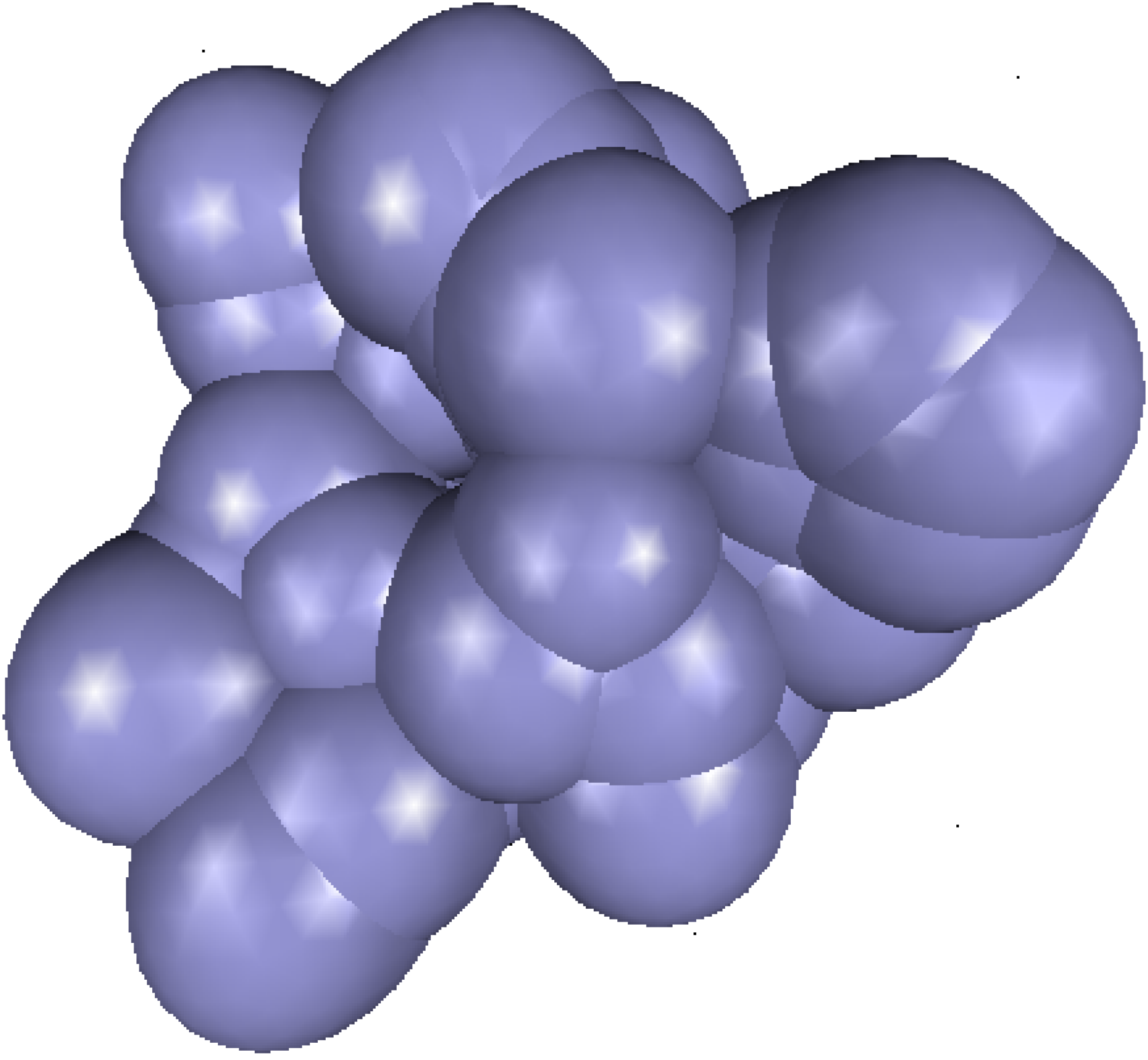
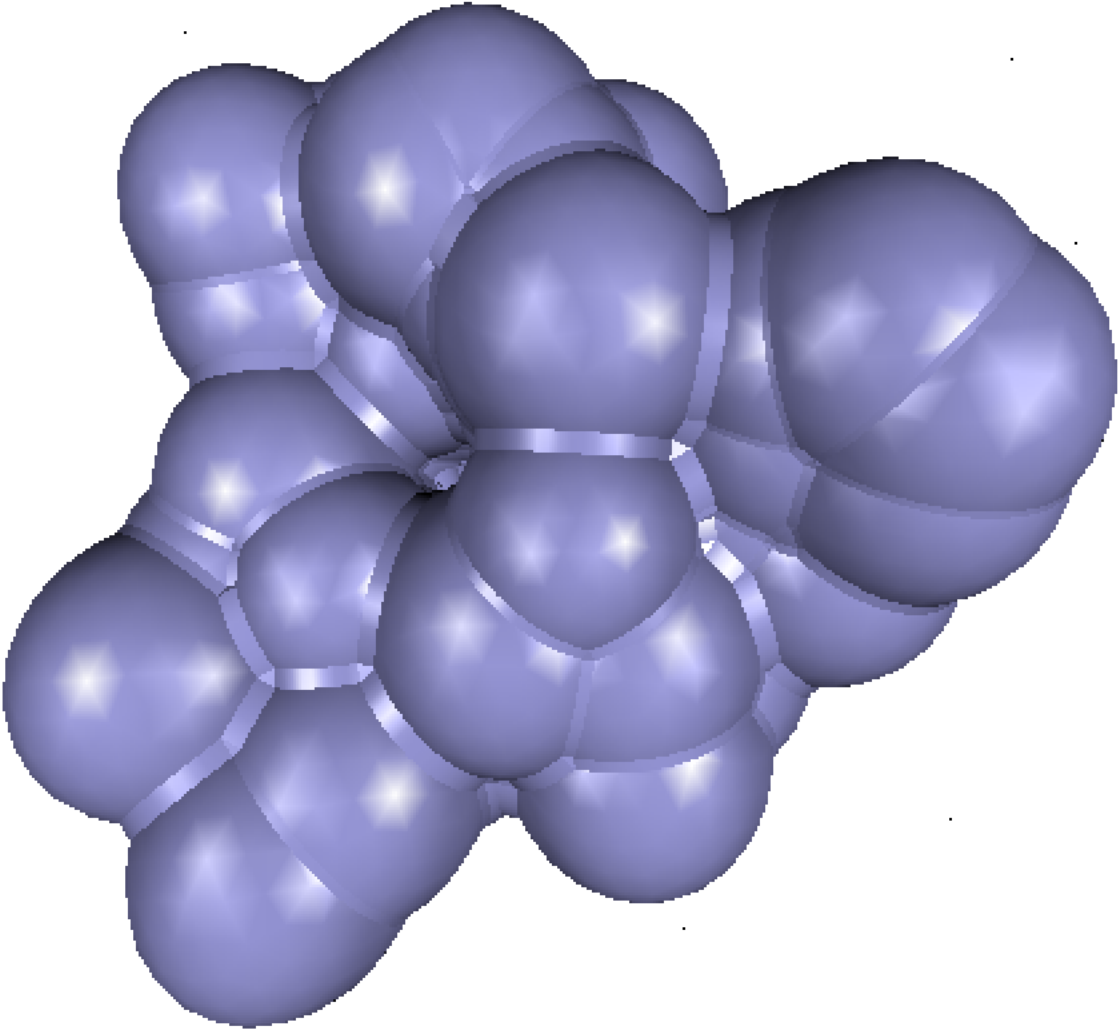
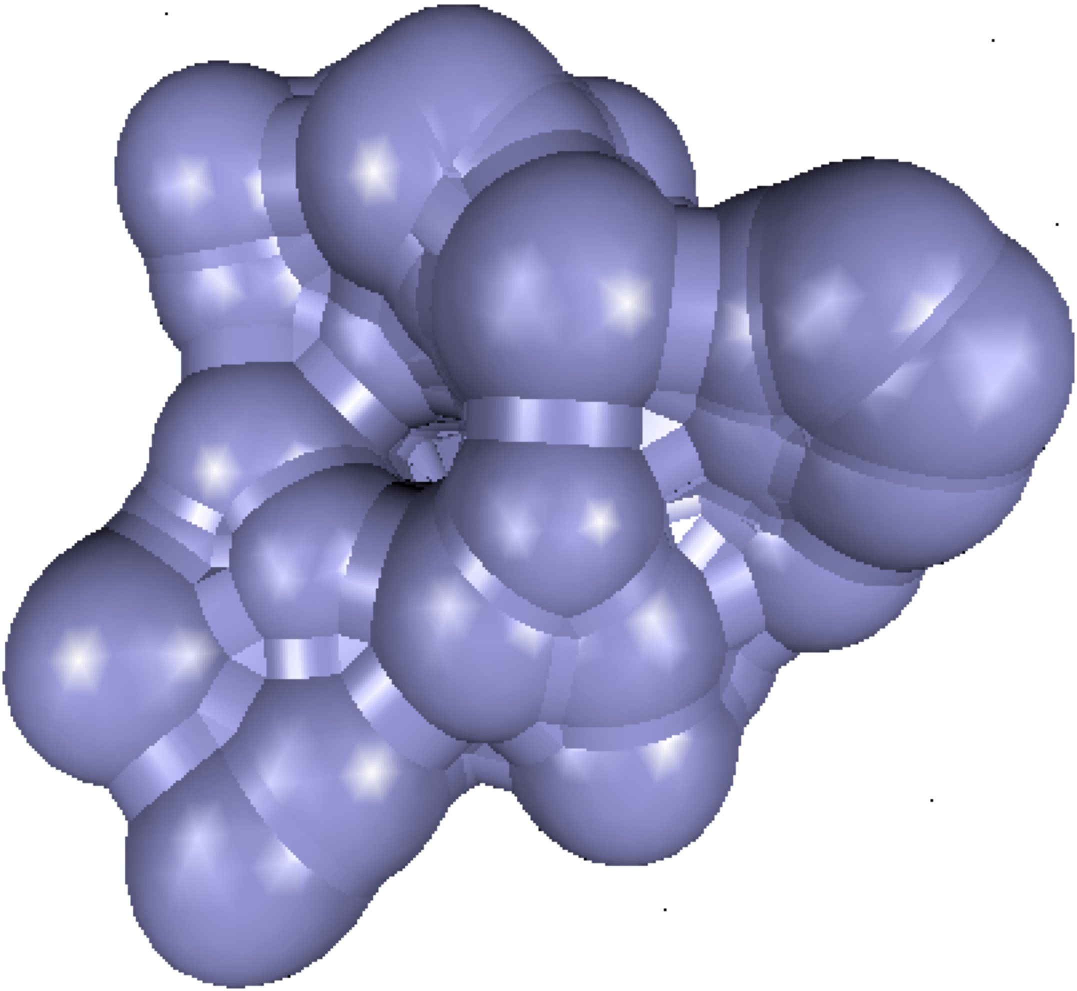
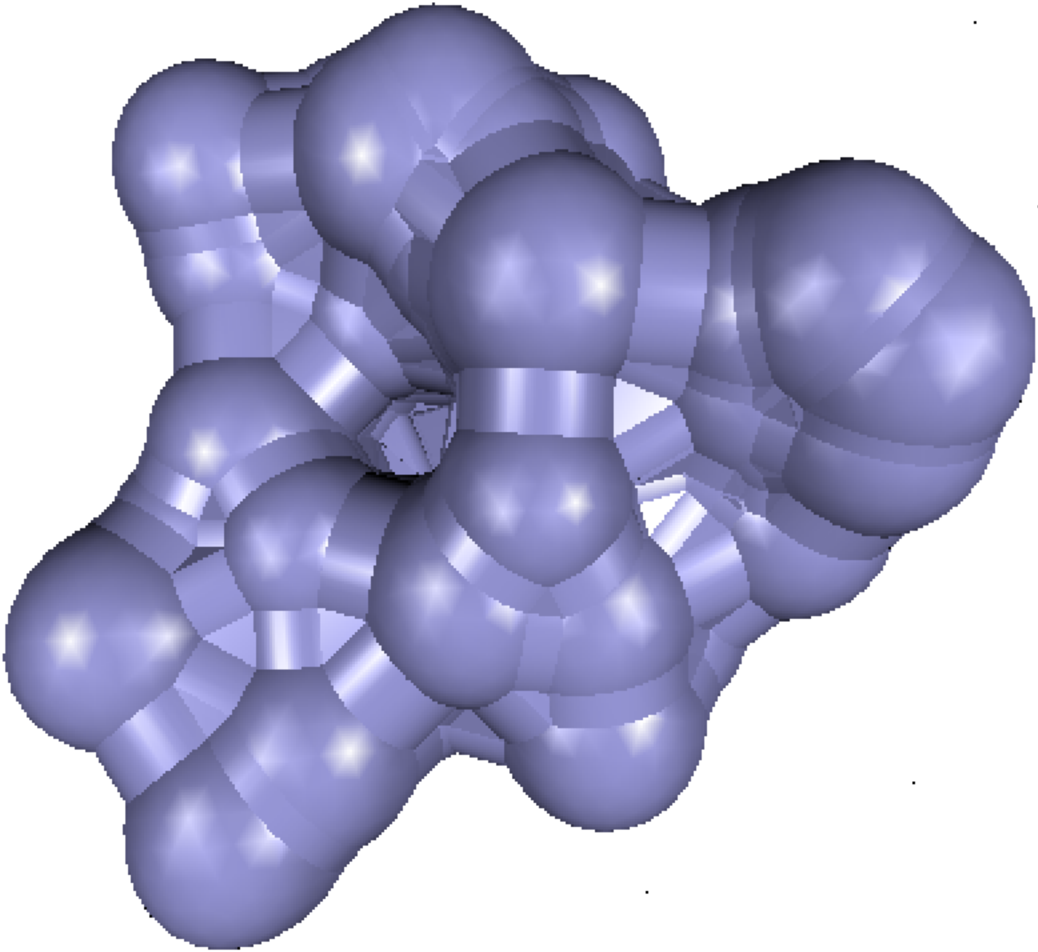
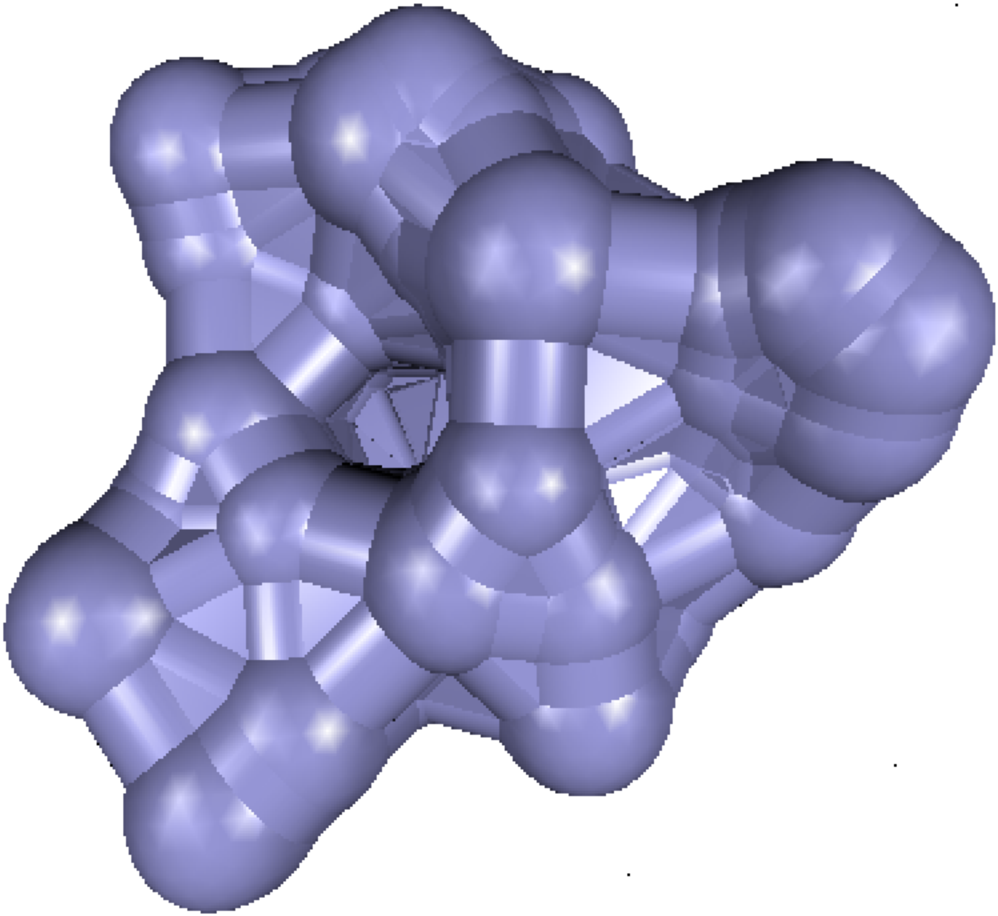
$\Longrightarrow$ $D_r(X)$ and $\bigcup_{x \in X} B_r(x)$ have same homotopy type

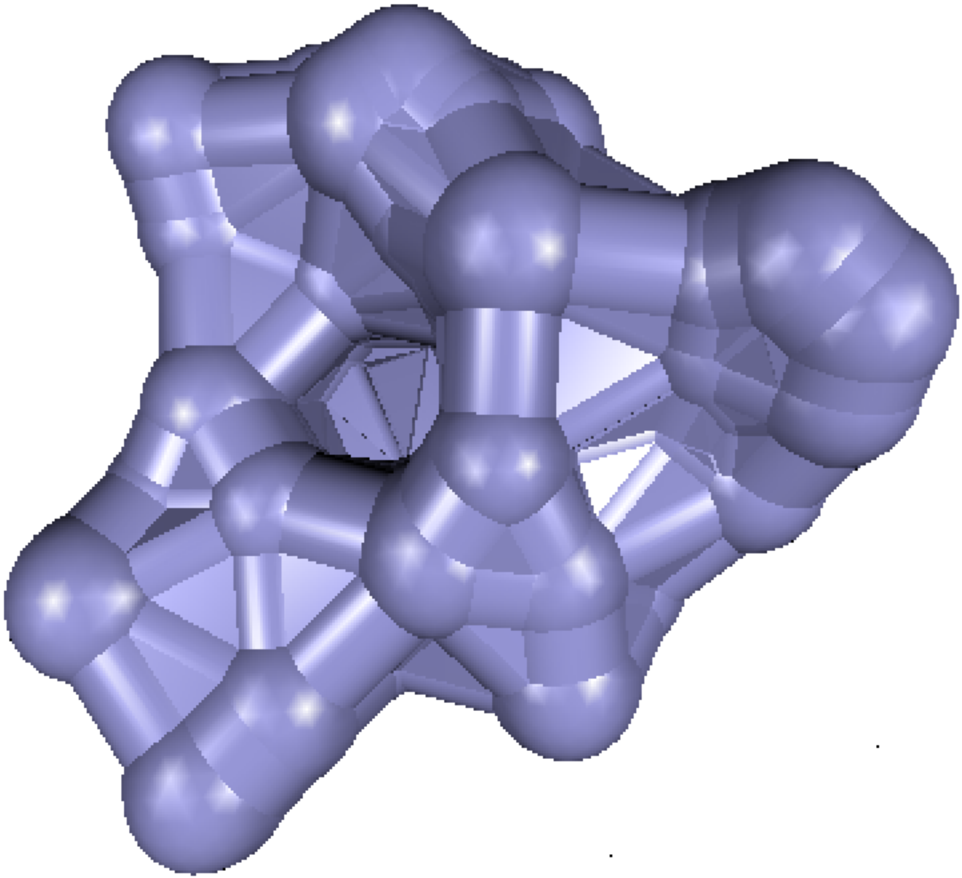


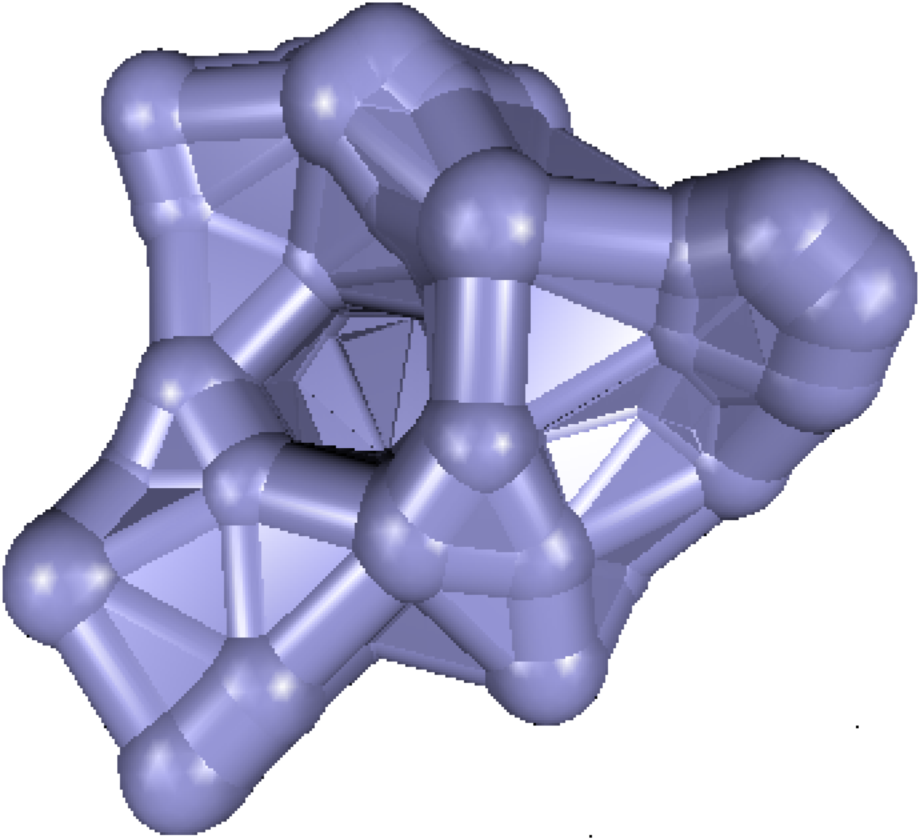


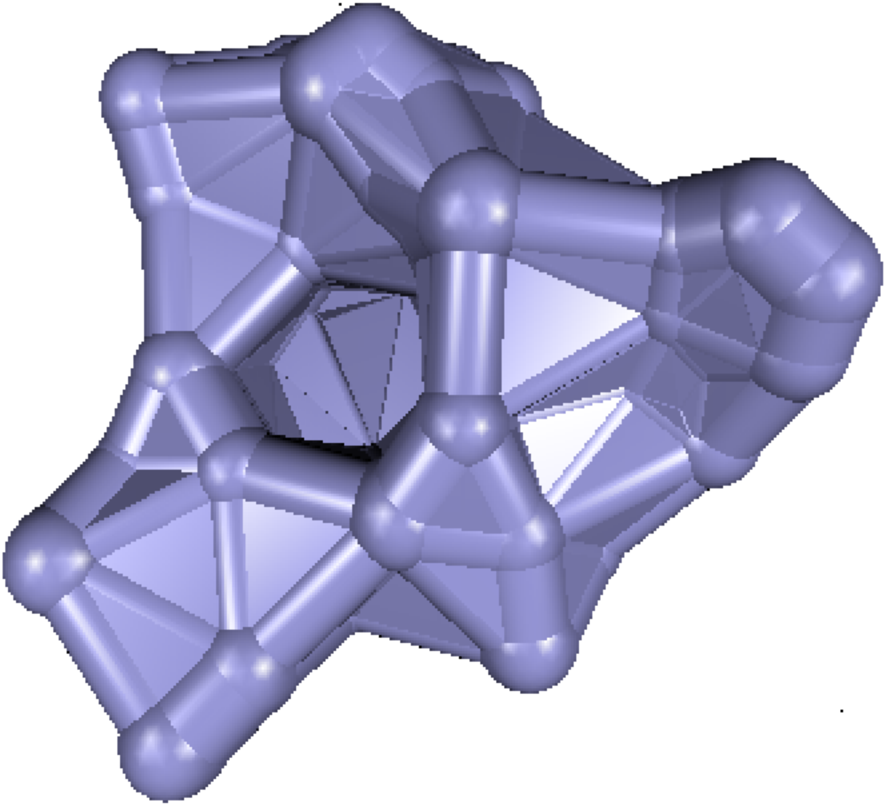


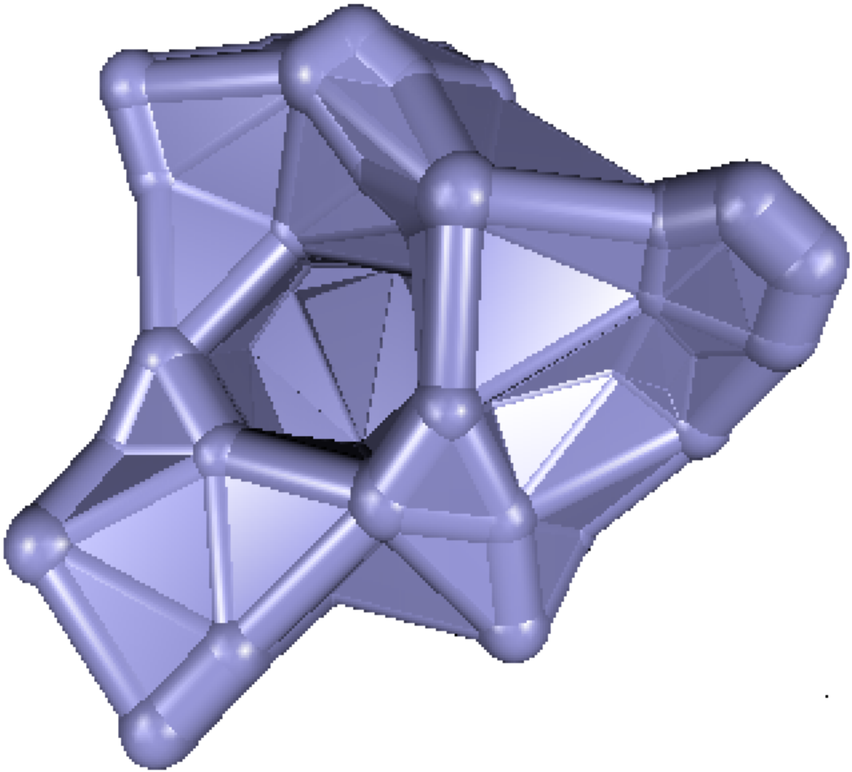


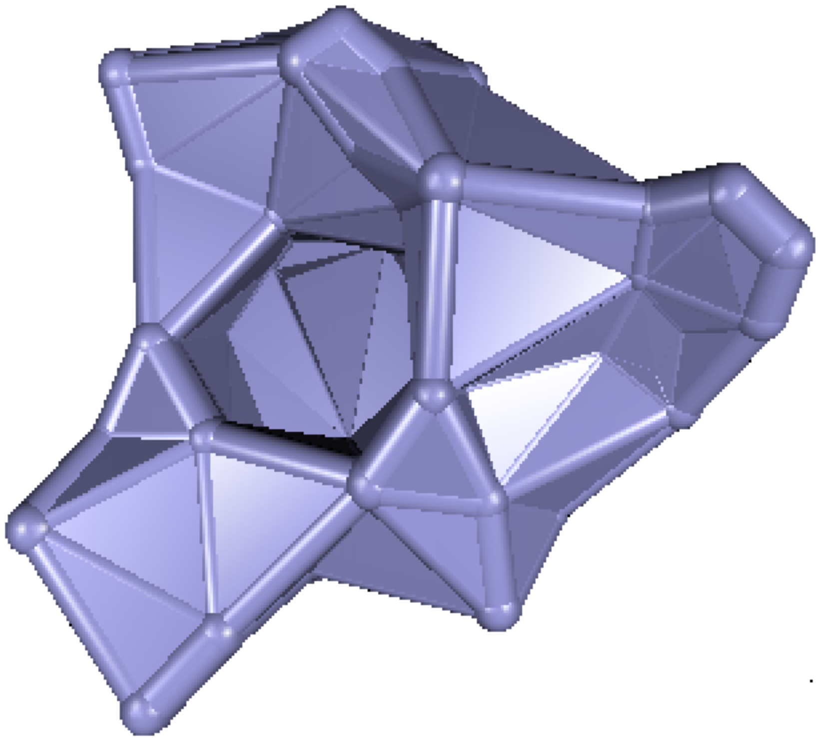


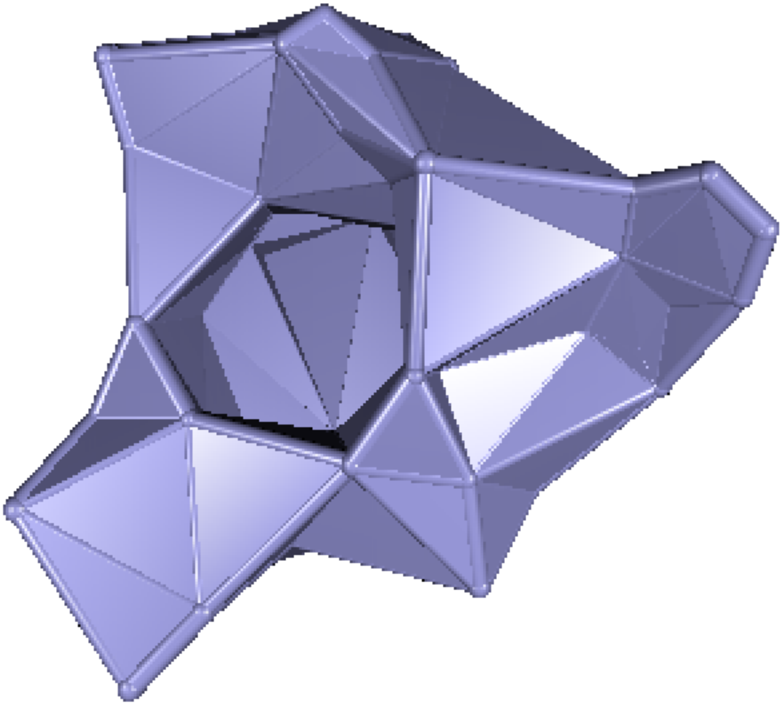


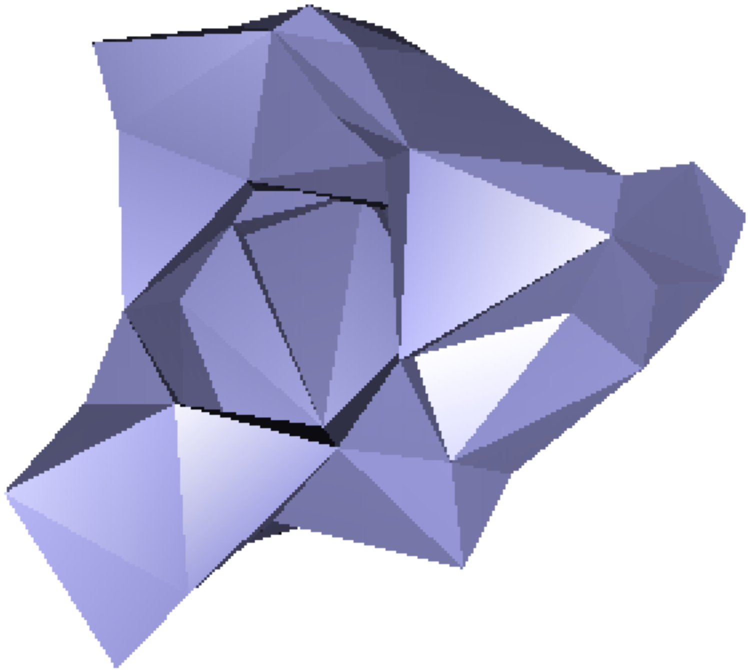












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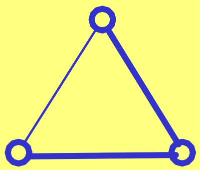
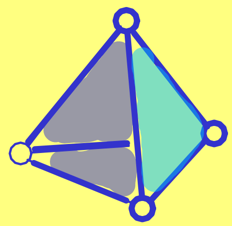
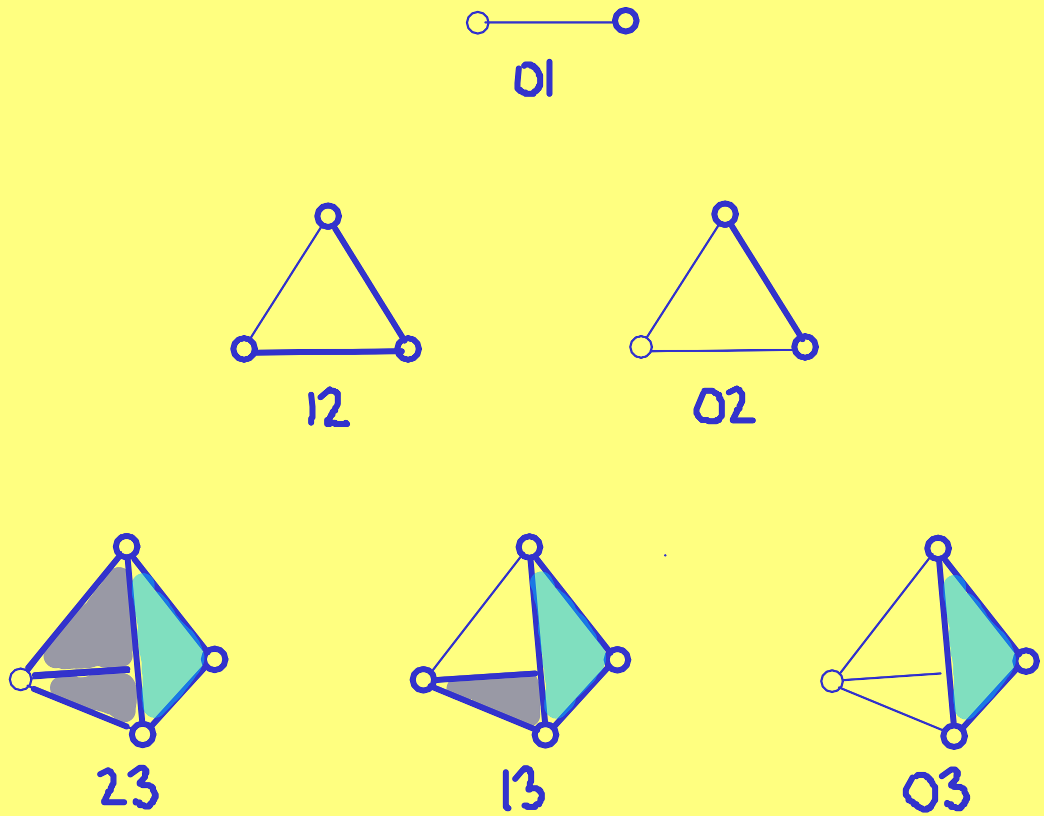
COLLAPSES



(elem.) collapse



Collapses



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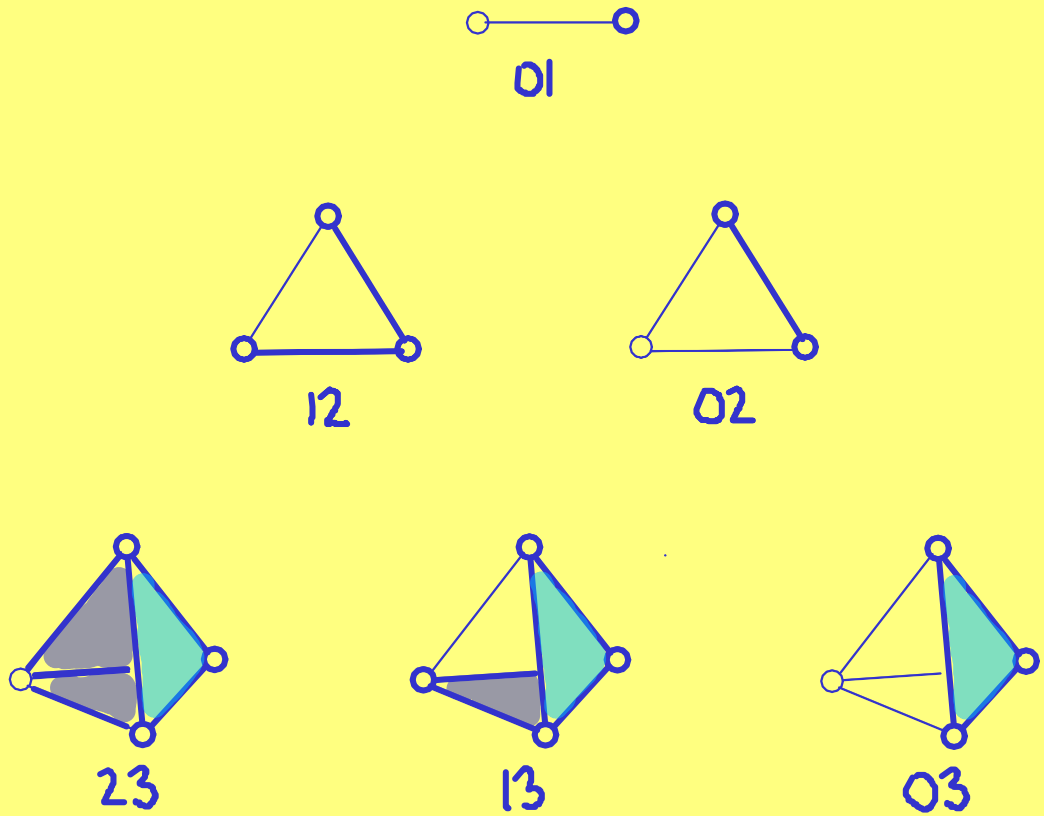
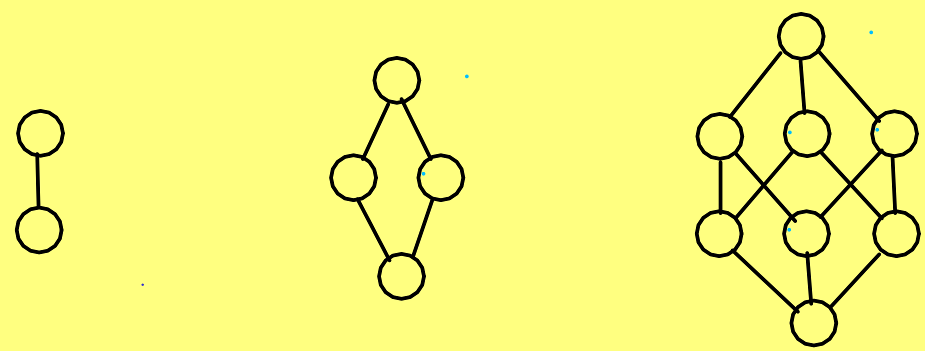


(elem.) collapse

interval

$[L,U] = \{L \subseteq Q \subseteq U\}$



Gen. Discrete Morse Function

gen. discrete vector field = partition into intervals

admits generalized discrete Morse function if acyclic

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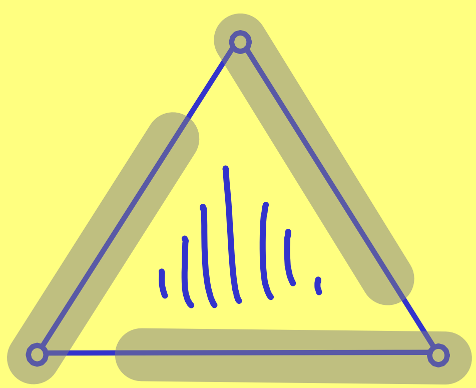

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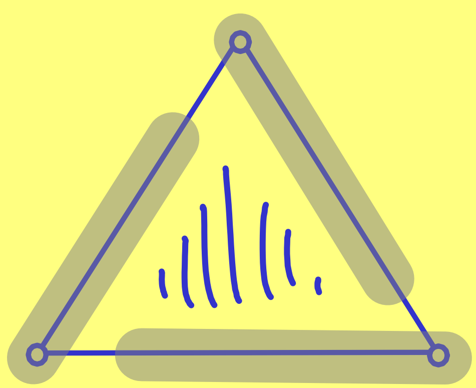

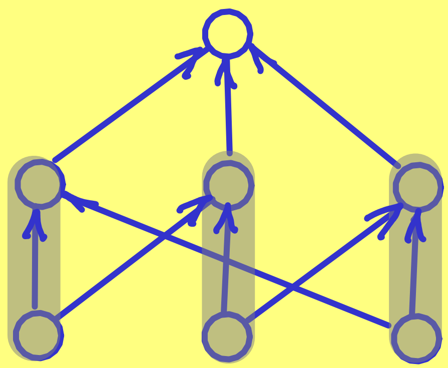

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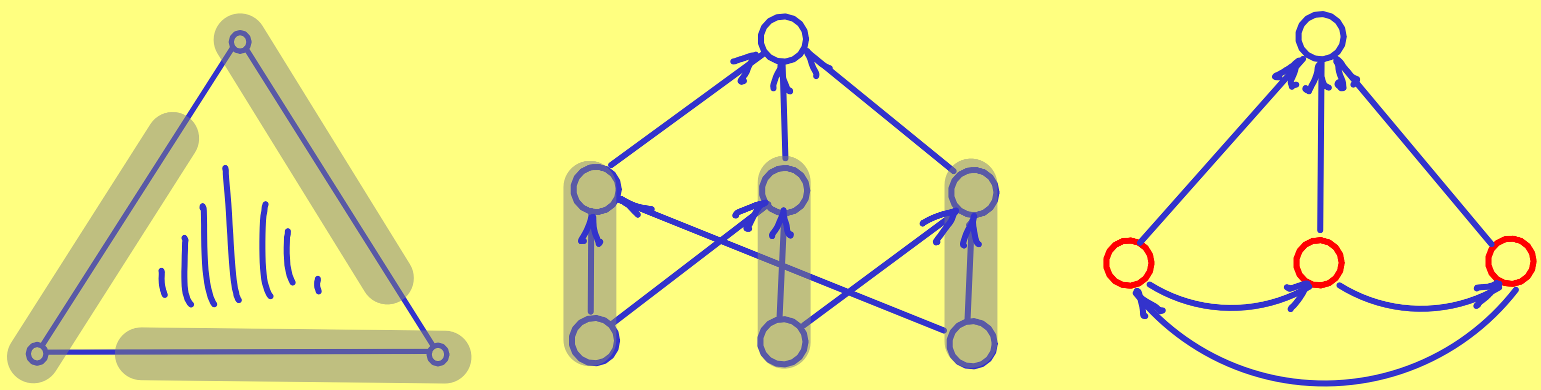

Wrap Complex

lower set of critical simplex, $Q\downarrow$

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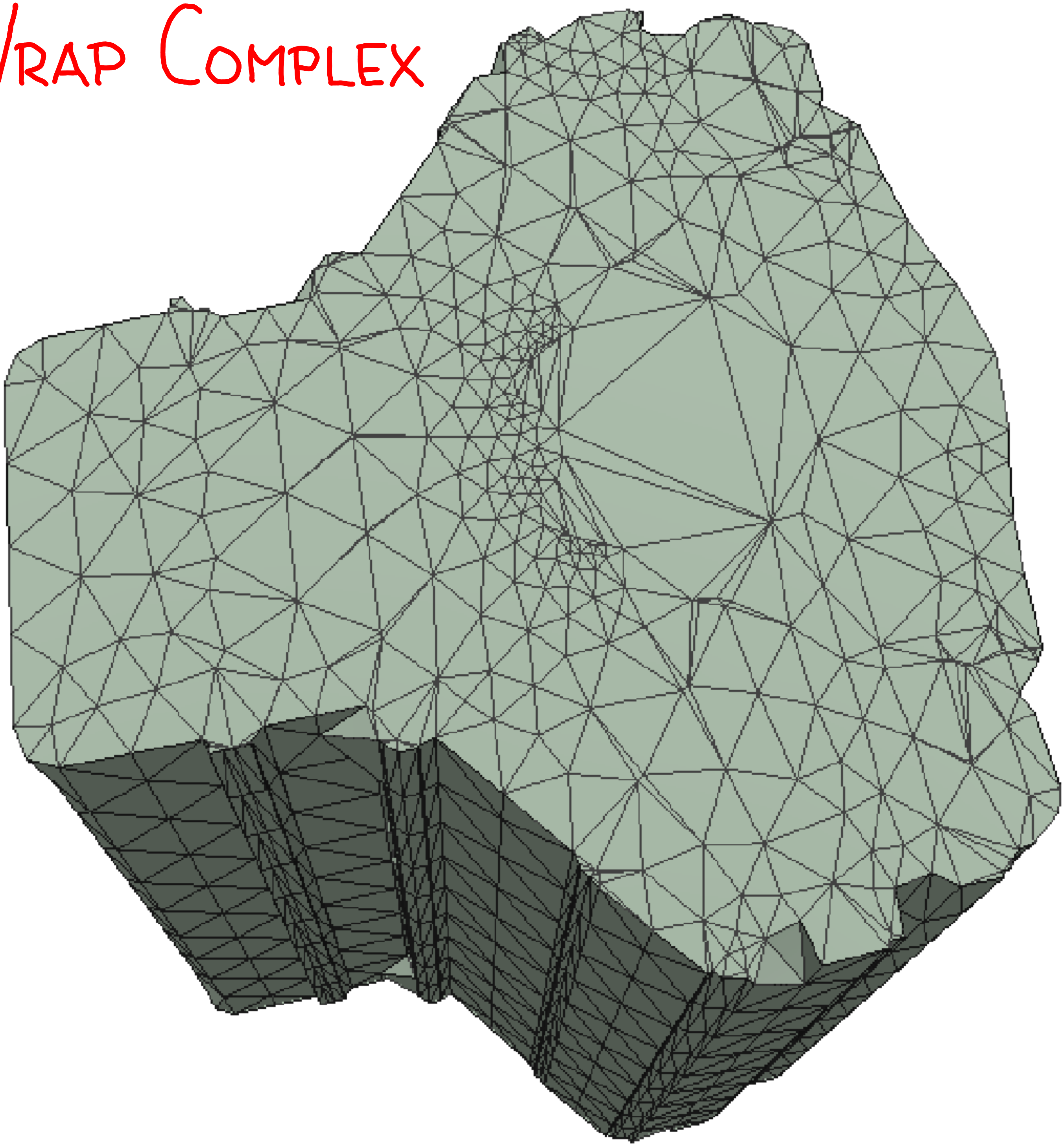
wrap complex for radius r is

$$\mathrm{Wrap}(r) = \bigcup_{R(Q) \leq r} Q\downarrow$$

[E. 1996]

Wrap Complex



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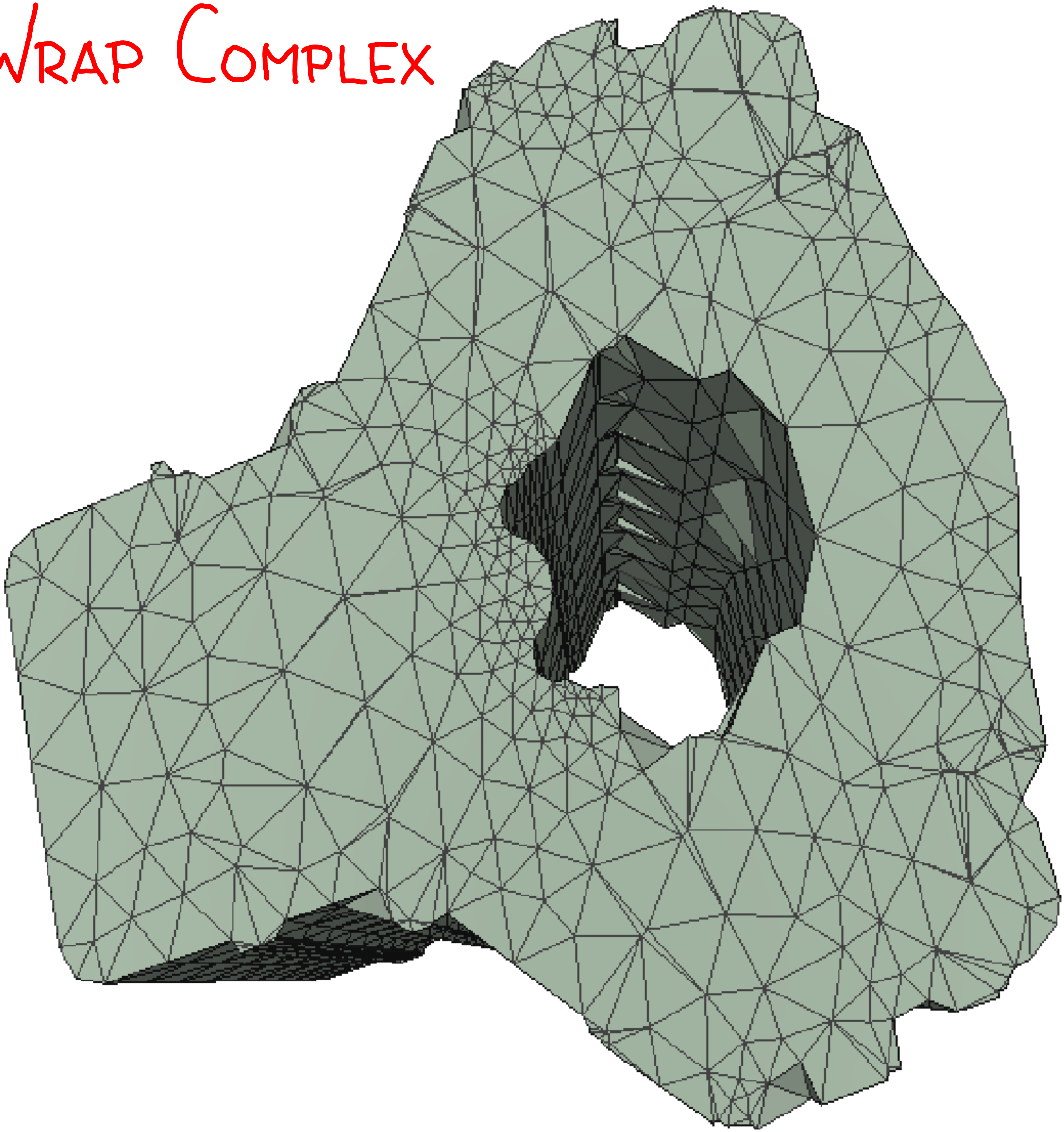

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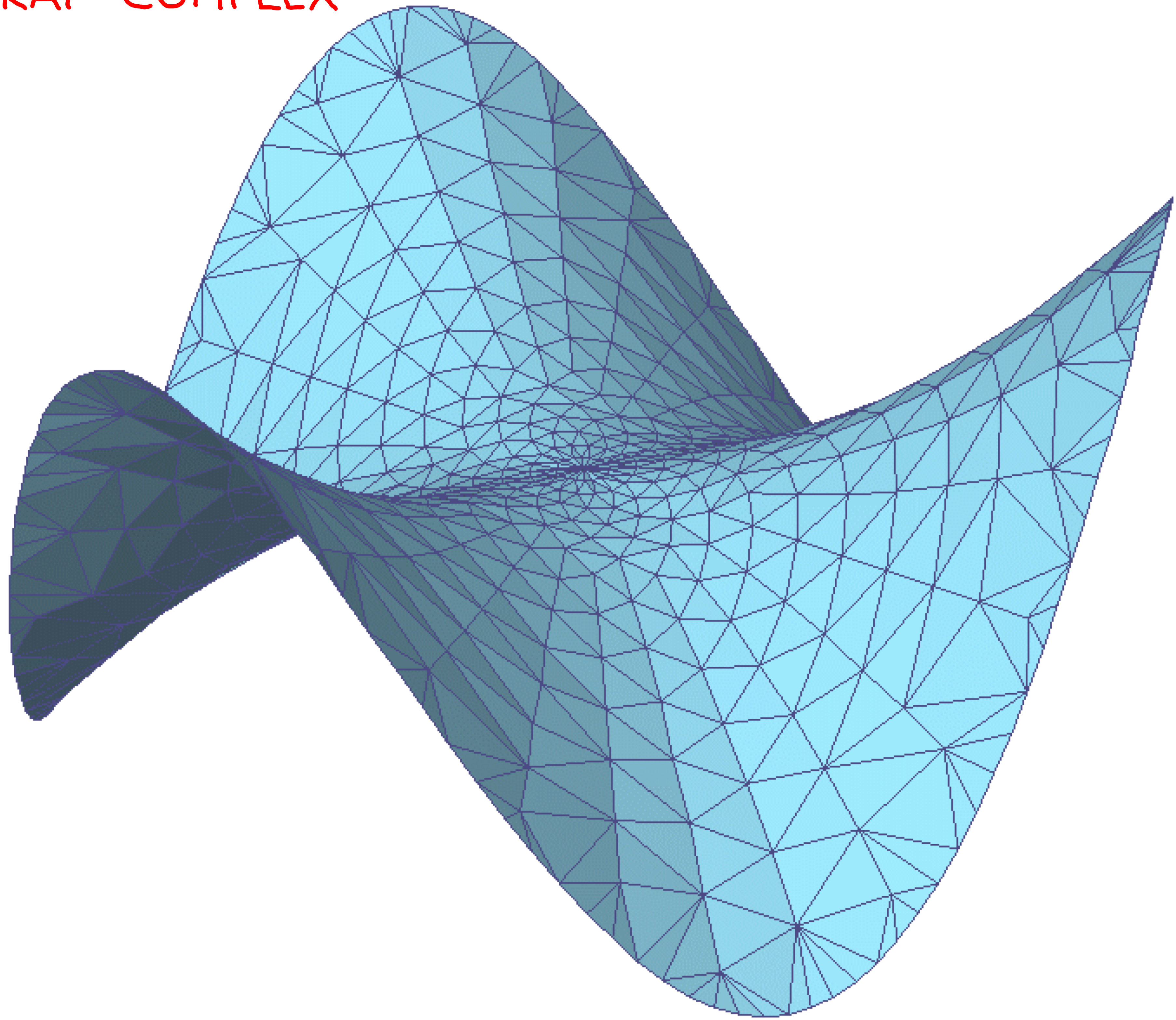
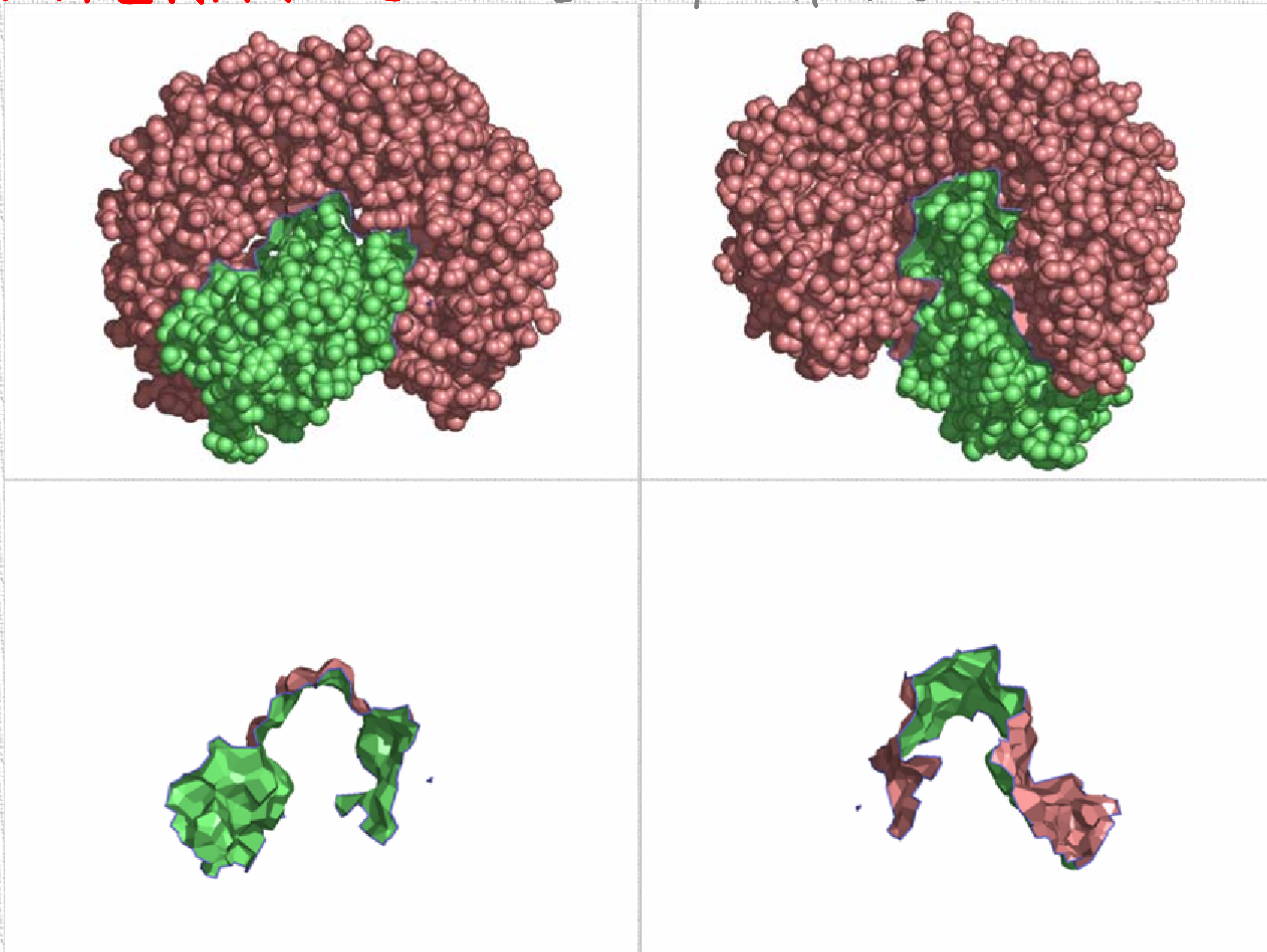
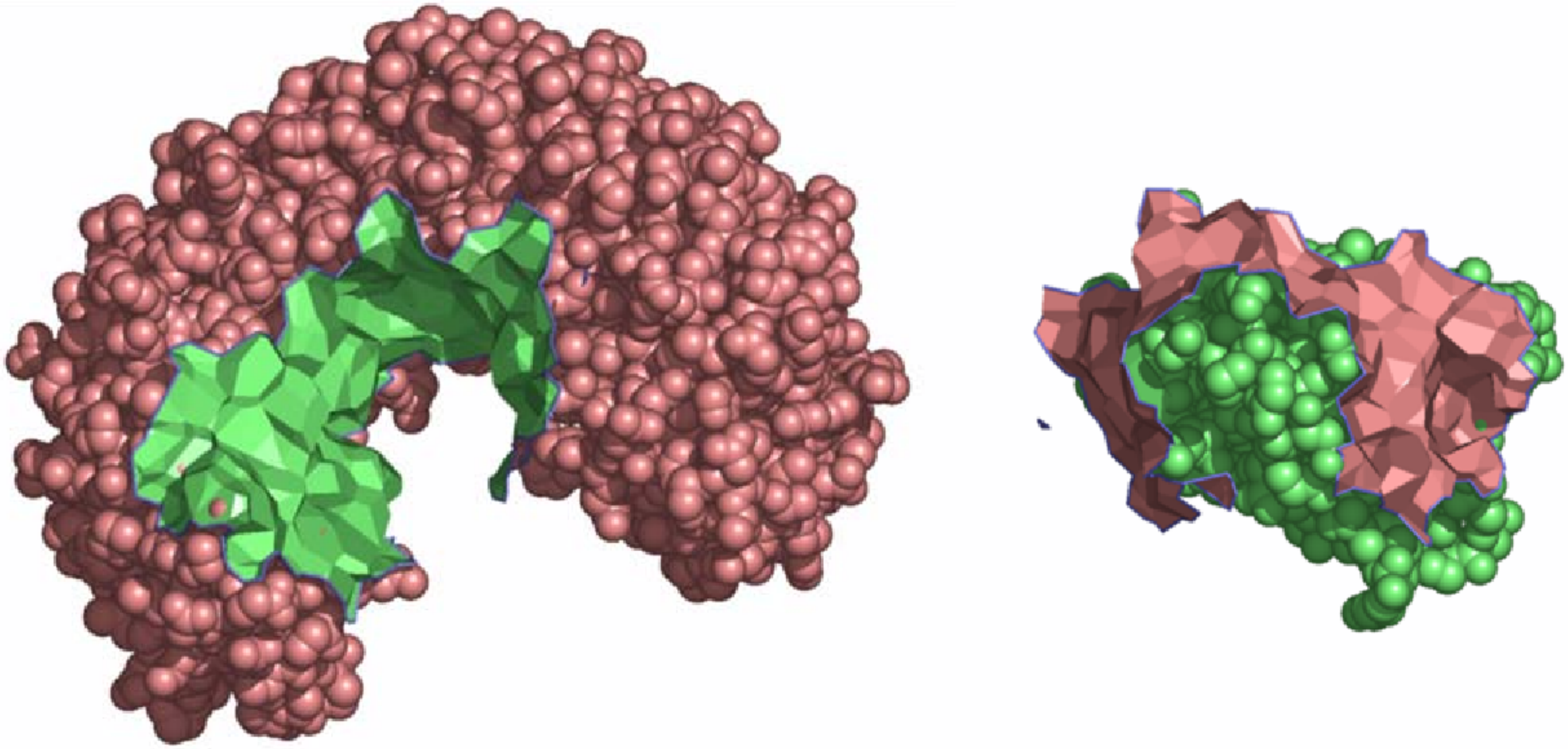


INTERFACES [BAN, E., RUDOLPH 2005]



Interfaces

[Ban, E., Rudolph 2005]



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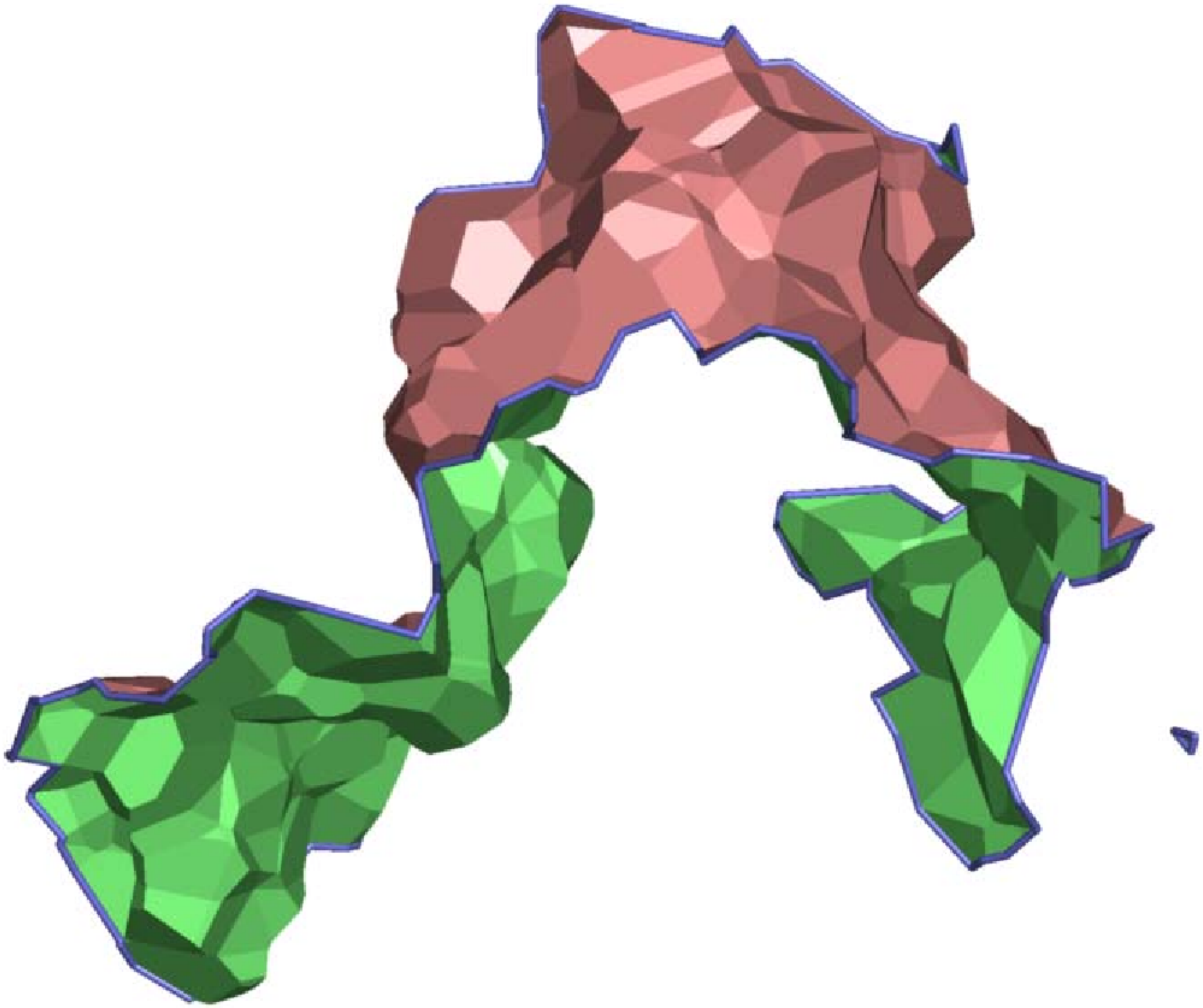

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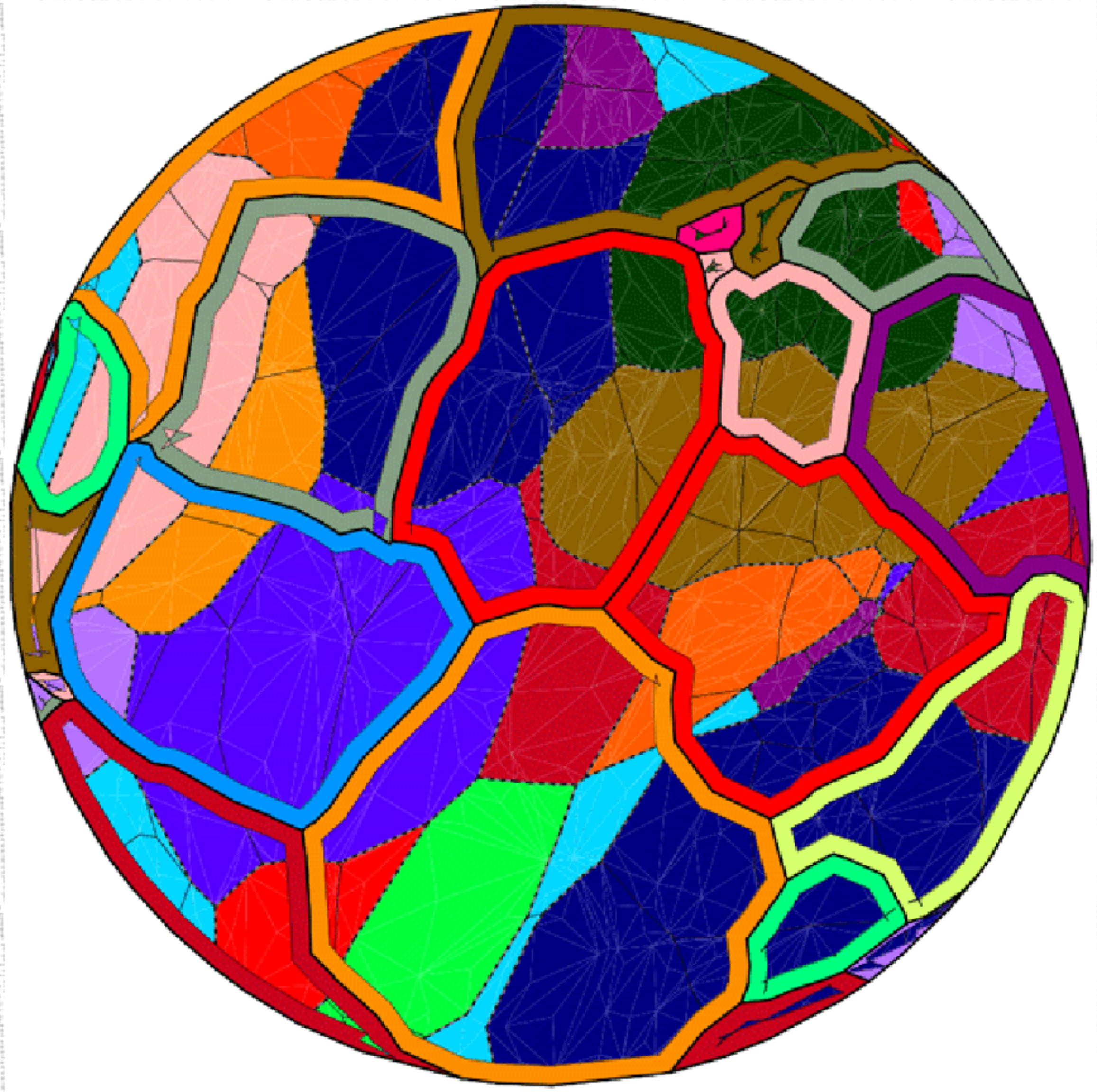

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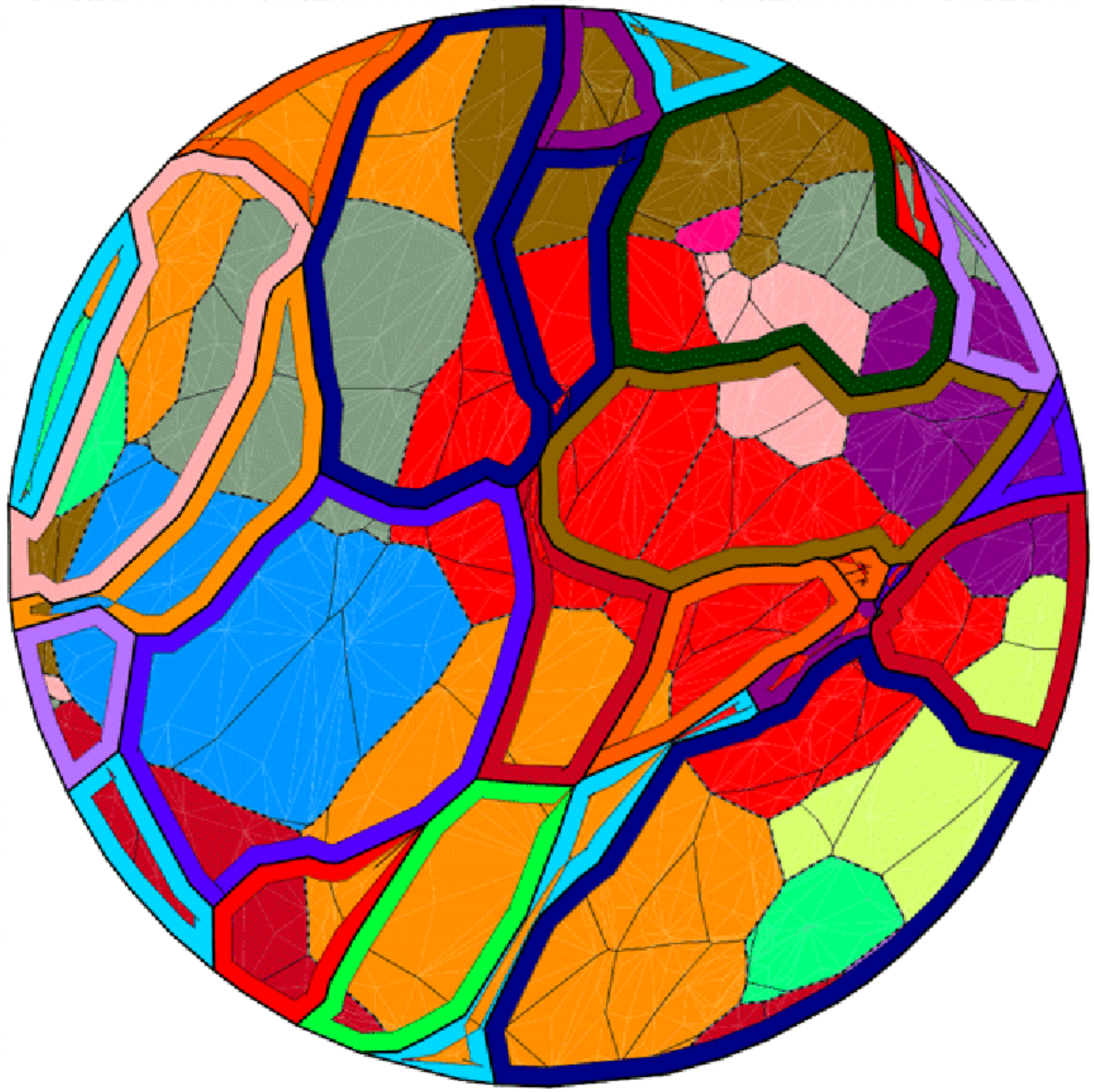

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Betti #s in $\mathbb{R}^3$:

β_0 = # components

β_1 = # tunnels

β_2 = # voids

BETTI #s in $\mathbb{R}^3$:

β_0 = #components

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VERTEX β_0++

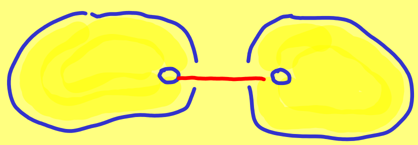
Betti #s in $\mathbb{R}^3$: β_0 = #components

β_1 = #tunnels

β_2 = #voids

Vertex  β_0^{++}

Edge



β_0^{--}

β_1^{++}

Betti #s

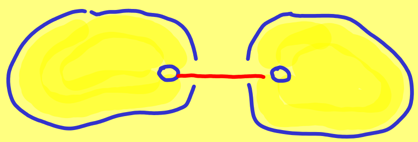
in $\mathbb{R}^3$: β_0 = # components

β_1 = # tunnels

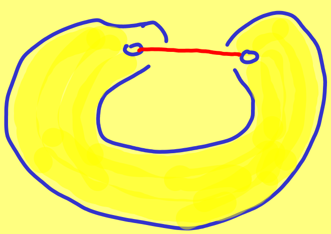
β_2 = # voids

VERTEX • β_0^{++}

EDGE

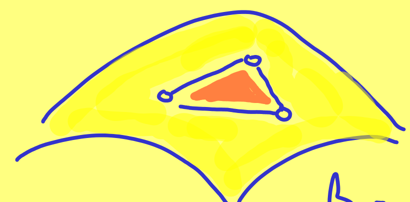


β_0^{--}



β_1^{++}

TRIANGLE



β_1^{--}

β_2^{++}

BETTI #s in $\mathbb{R}^3$:

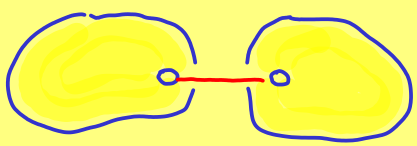
β_0 = #components

β_1 = #tunnels

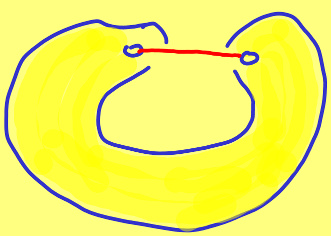
β_2 = #voids

VERTEX • β_0++

EDGE

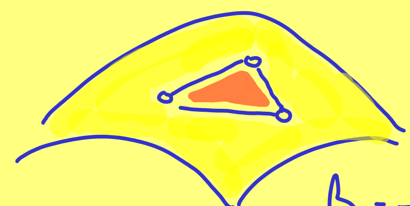


β_0--



β_1++

TRIANGLE



β_1--

β_2++

TETRAHEDRON β_2--

Incremental Algorithm

$\beta_0 = \beta_1 = \ldots = \beta_n = 0;$

for $i = 1$ to m do

  $k = \dim Q_i;$

  if $Q_i \in k$-cycle then β_i++

            else β_{i-1}--

  endif

endfor

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$\beta_0 = \beta_1 = \ldots = \beta_n = 0;$

for $i = 1$ to m do

  $k = \dim Q_i;$

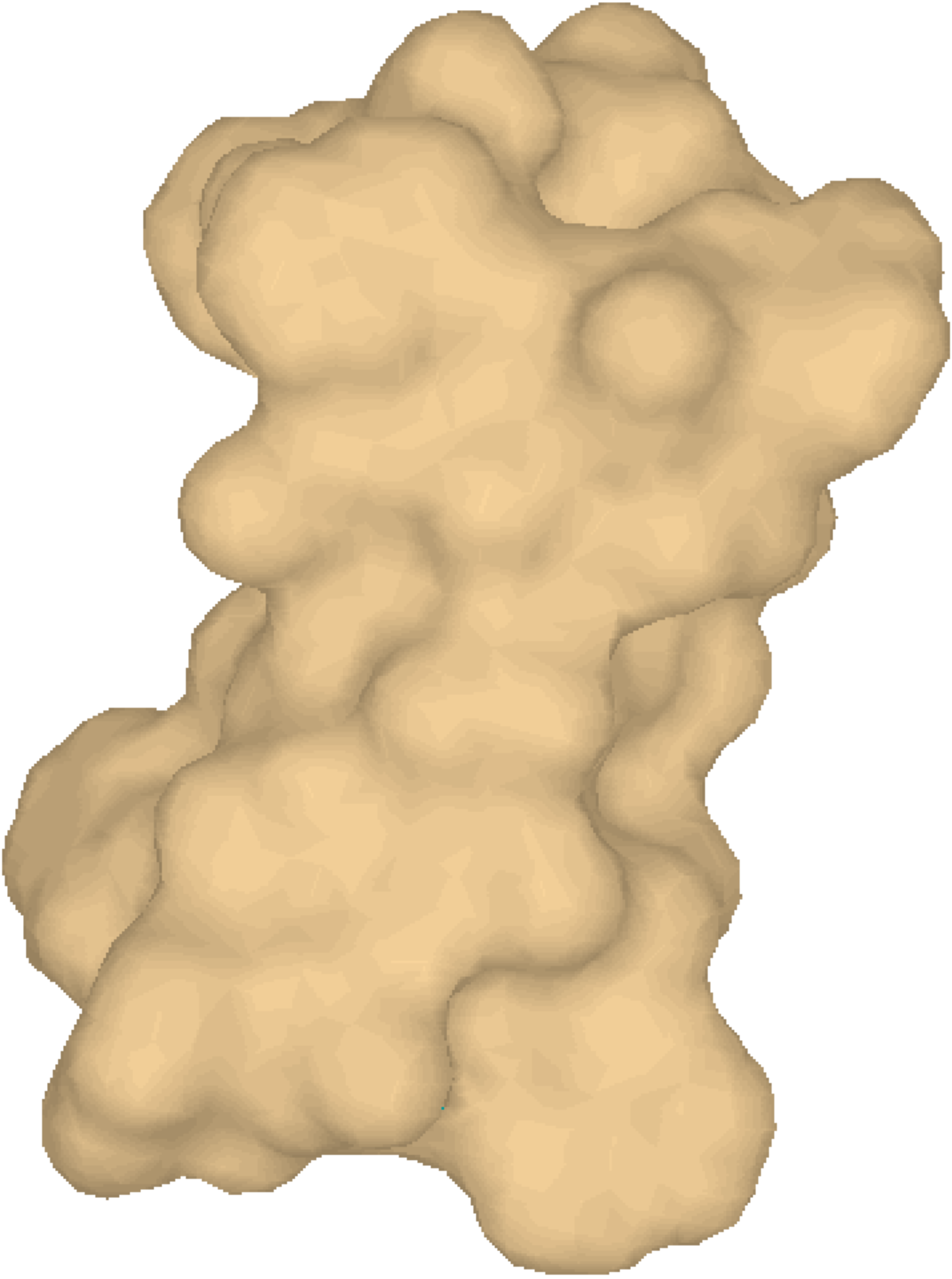
  if $Q_i \in k$-cycle then β_i++ (birth)

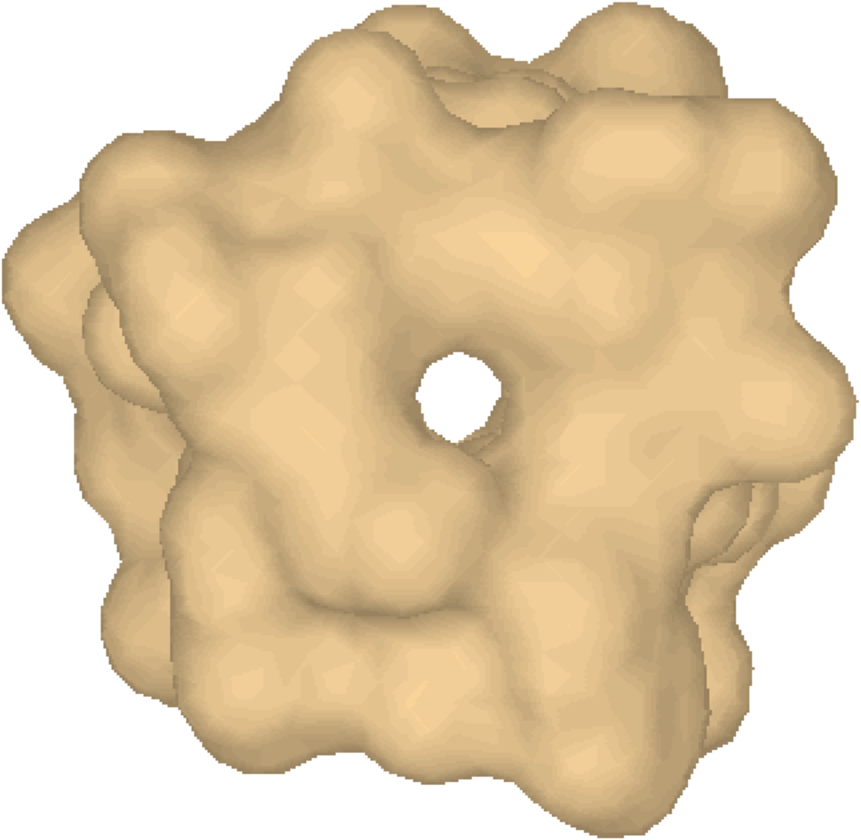
  else β_{i-1}-- (death)

  endif

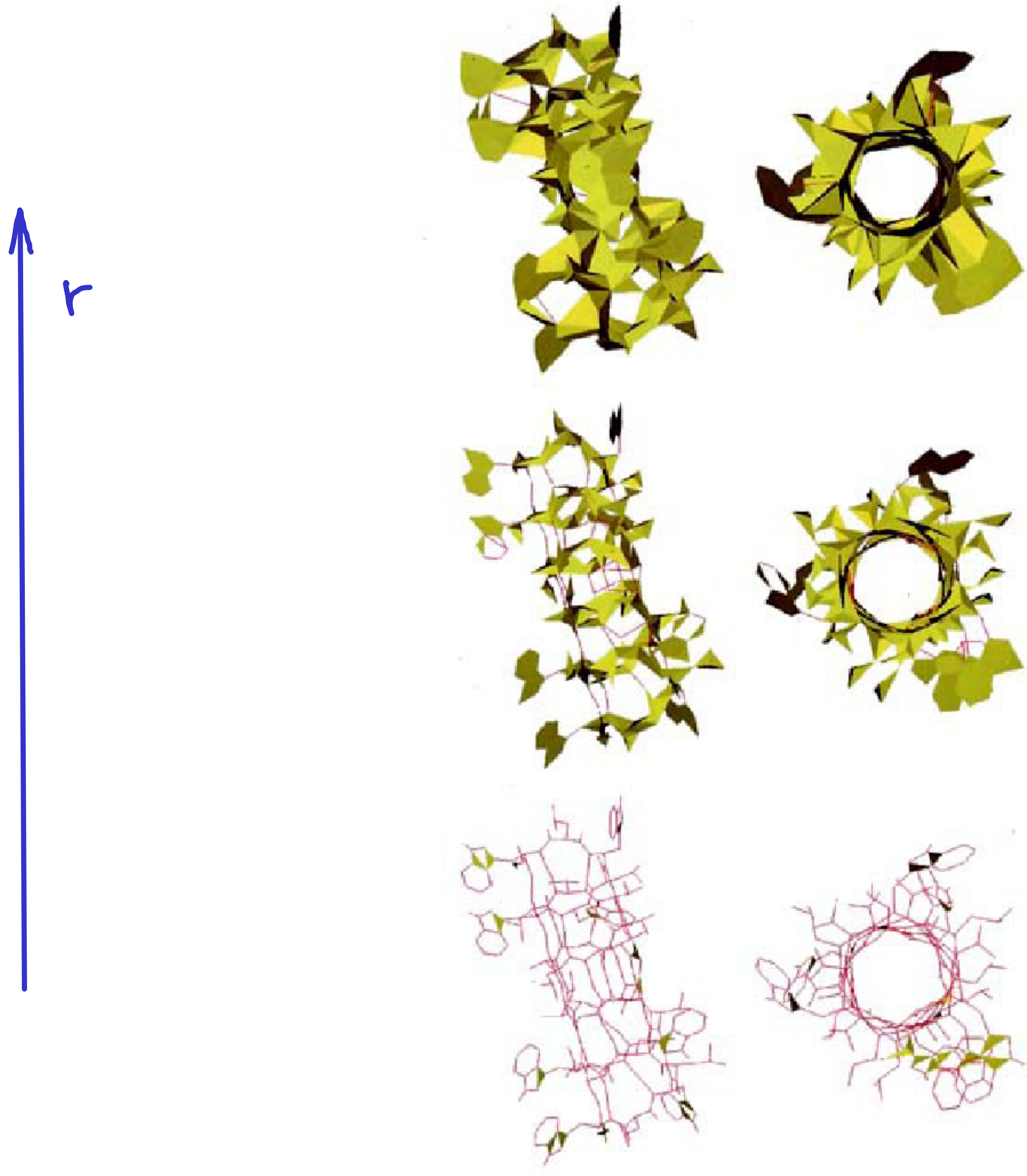
endfor

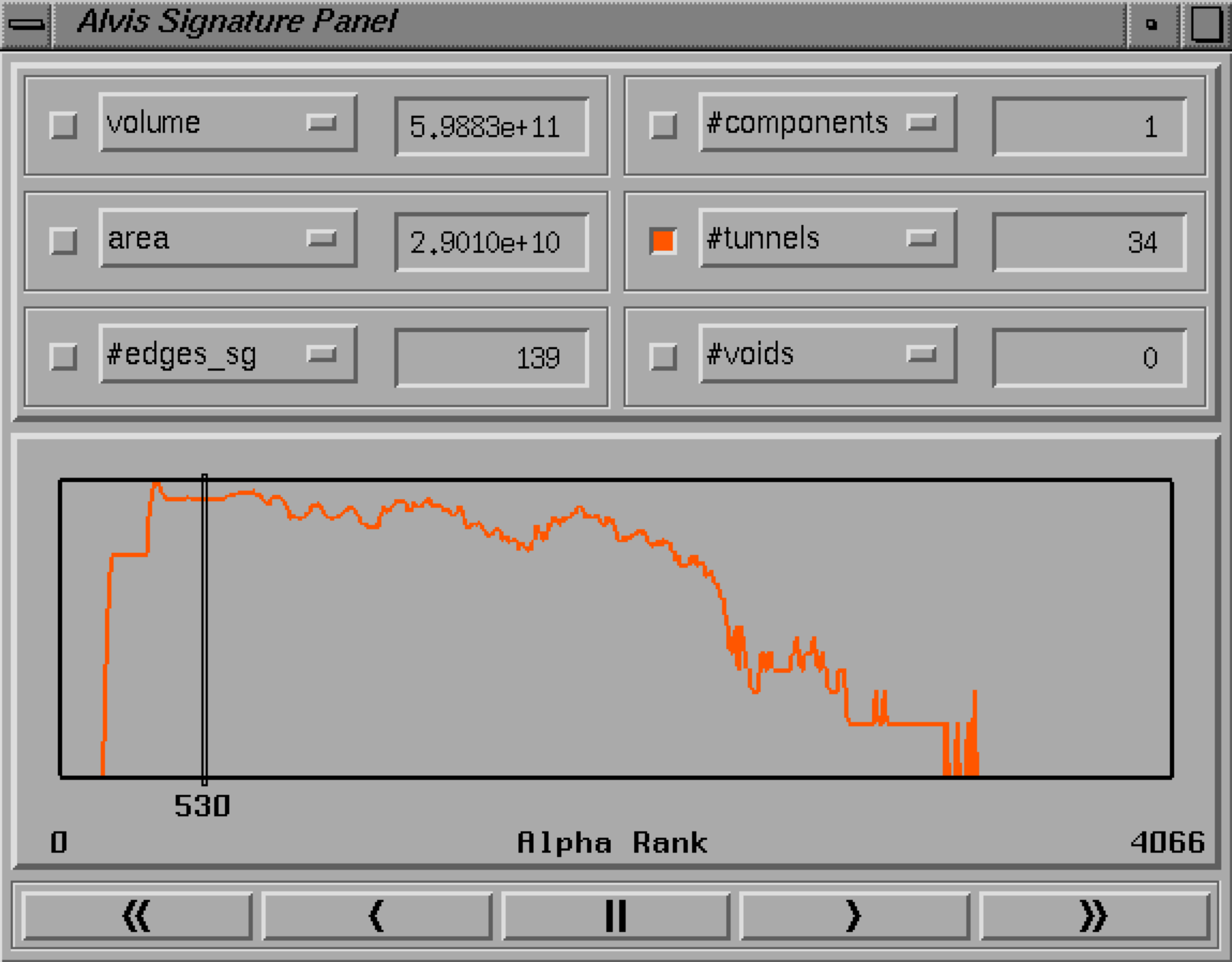
[Delfinado, E. 1995]





Number of Tunnels




Alvis Signature Panel
volume
5.9883e+11
#components
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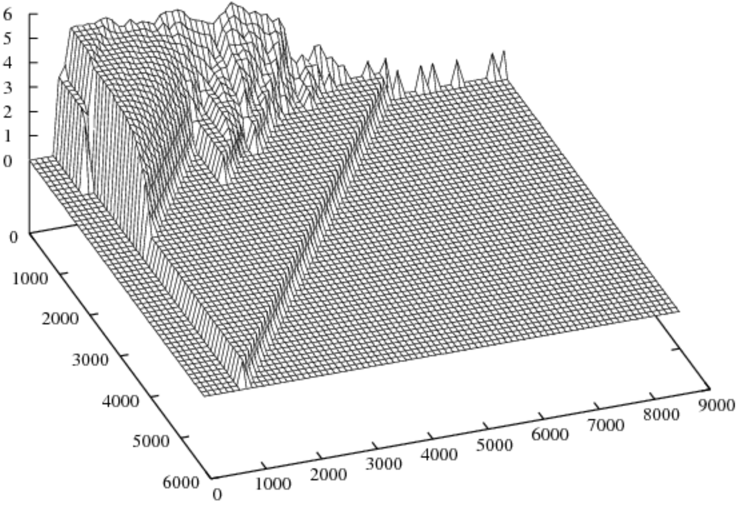
area
2.9010e+10
#tunnels
34
#edges_sg
139
#voids
0
530
0
Alpha Rank
4066



6
5
4
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1
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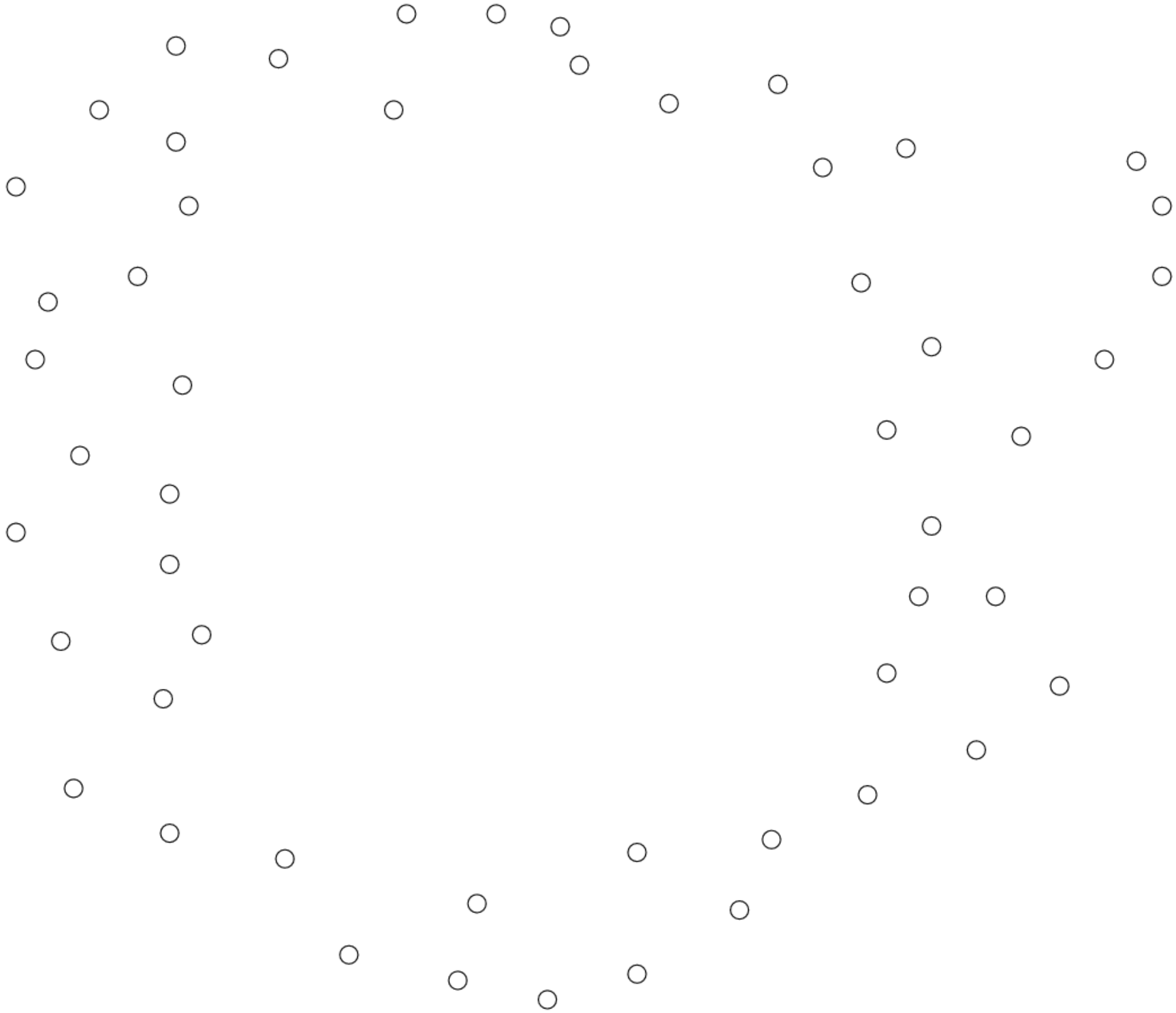
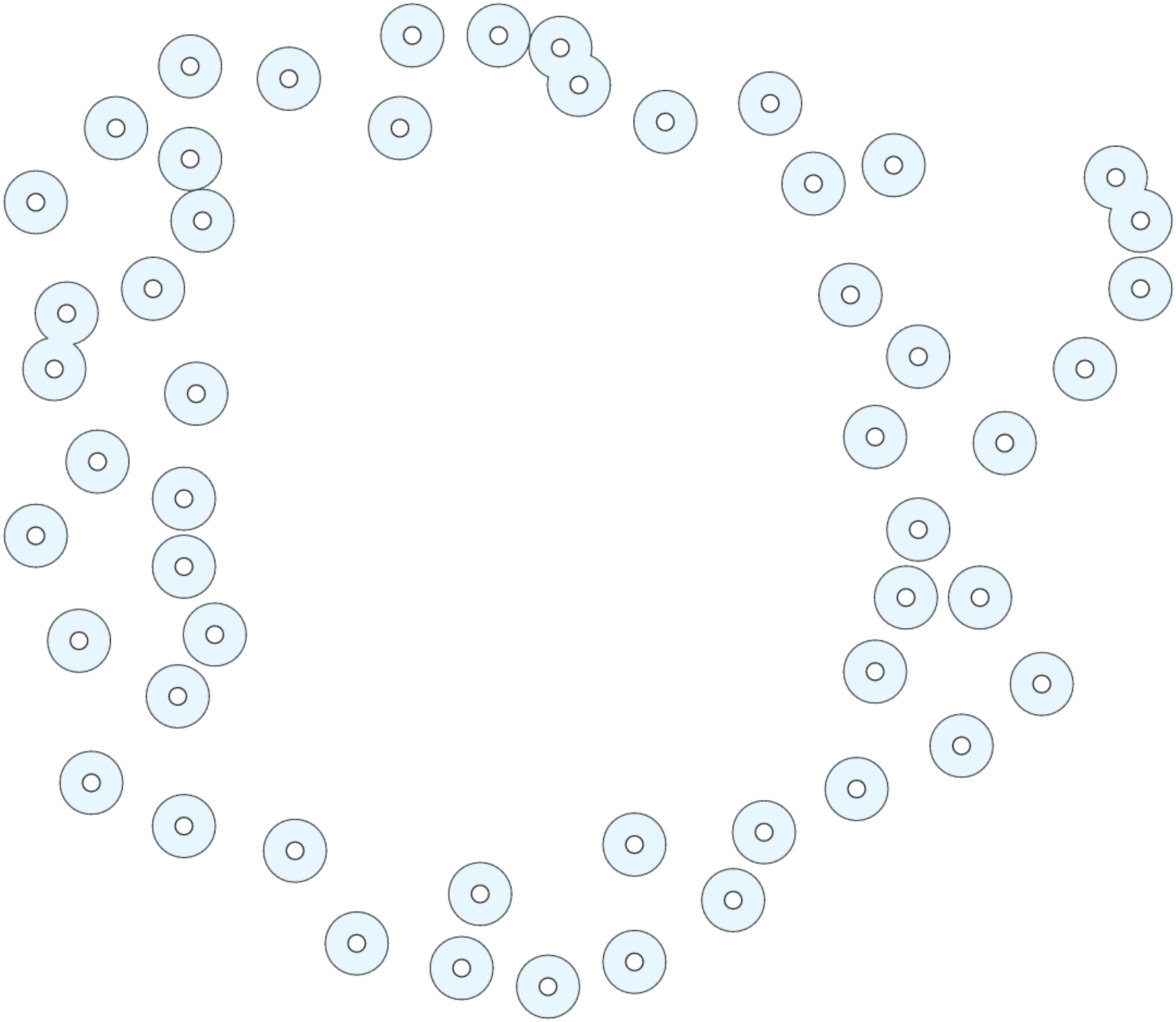
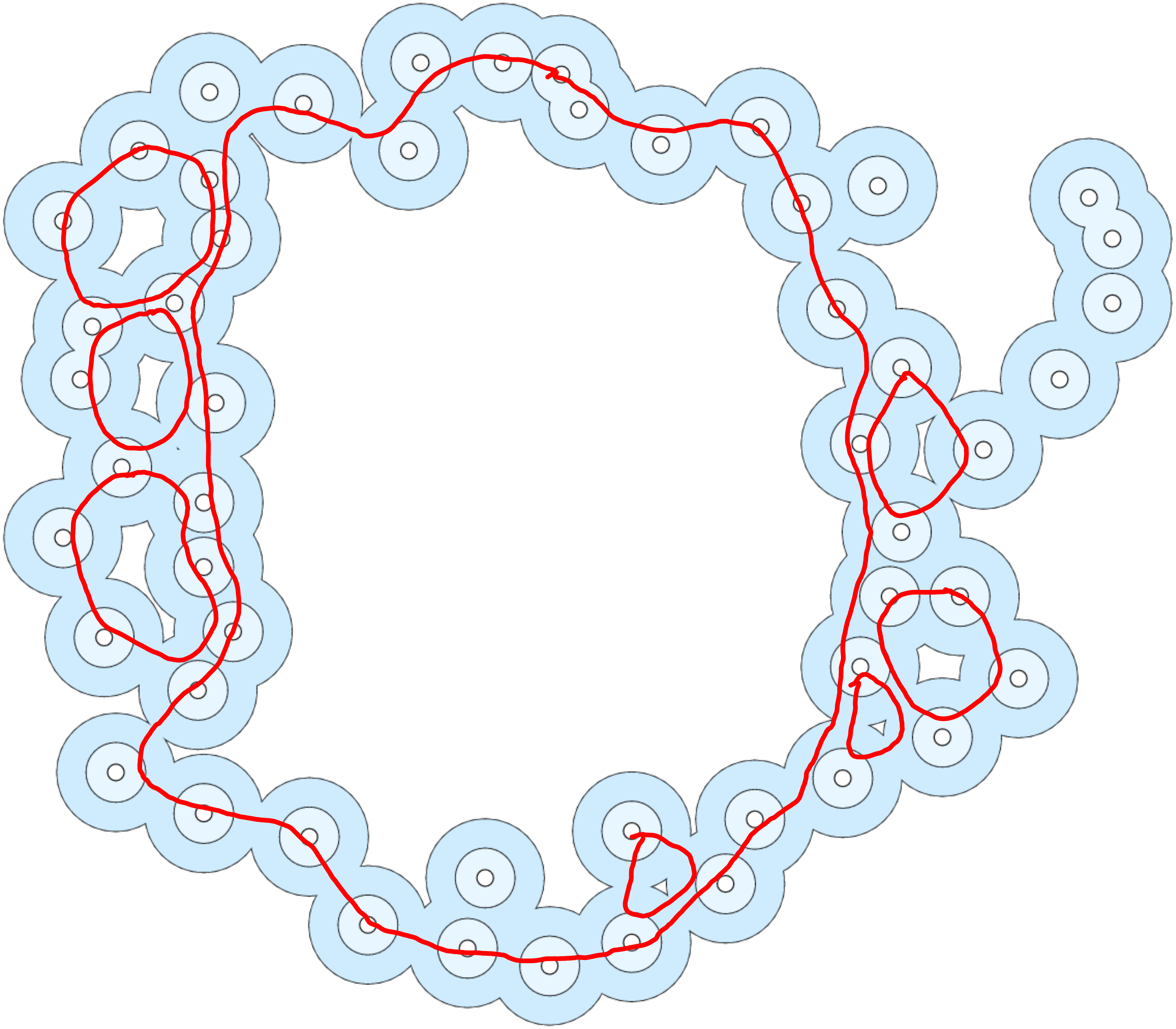
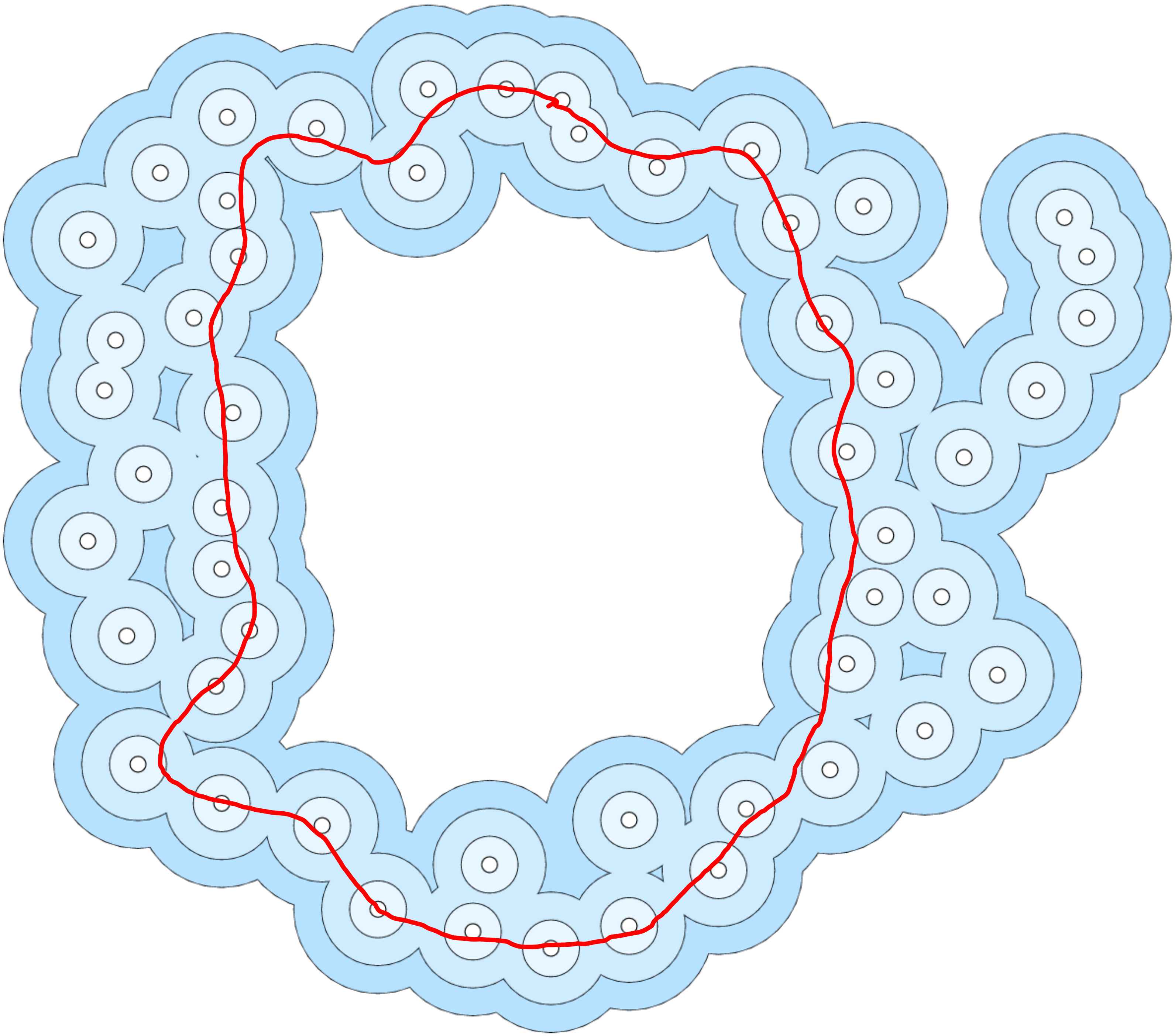
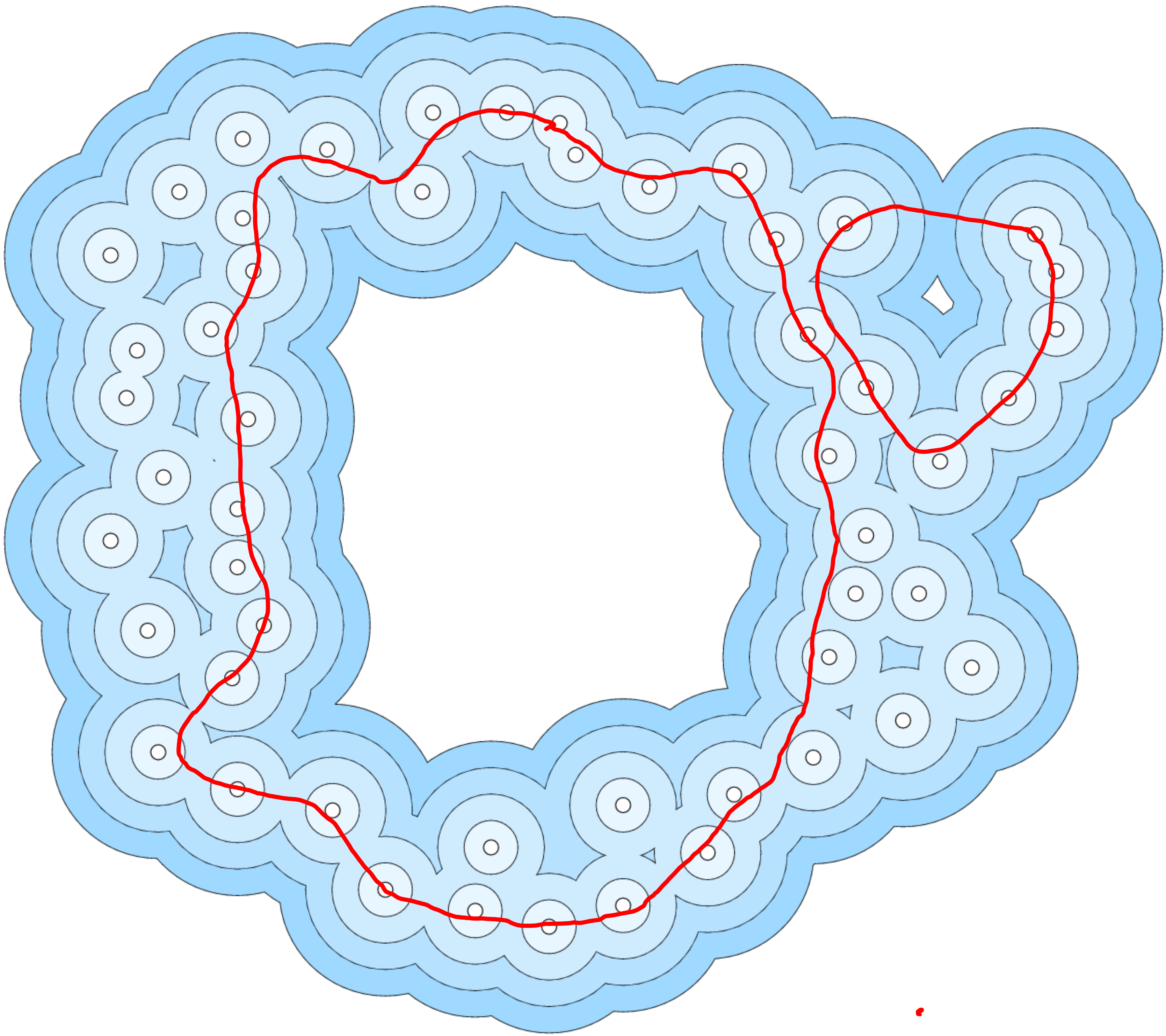
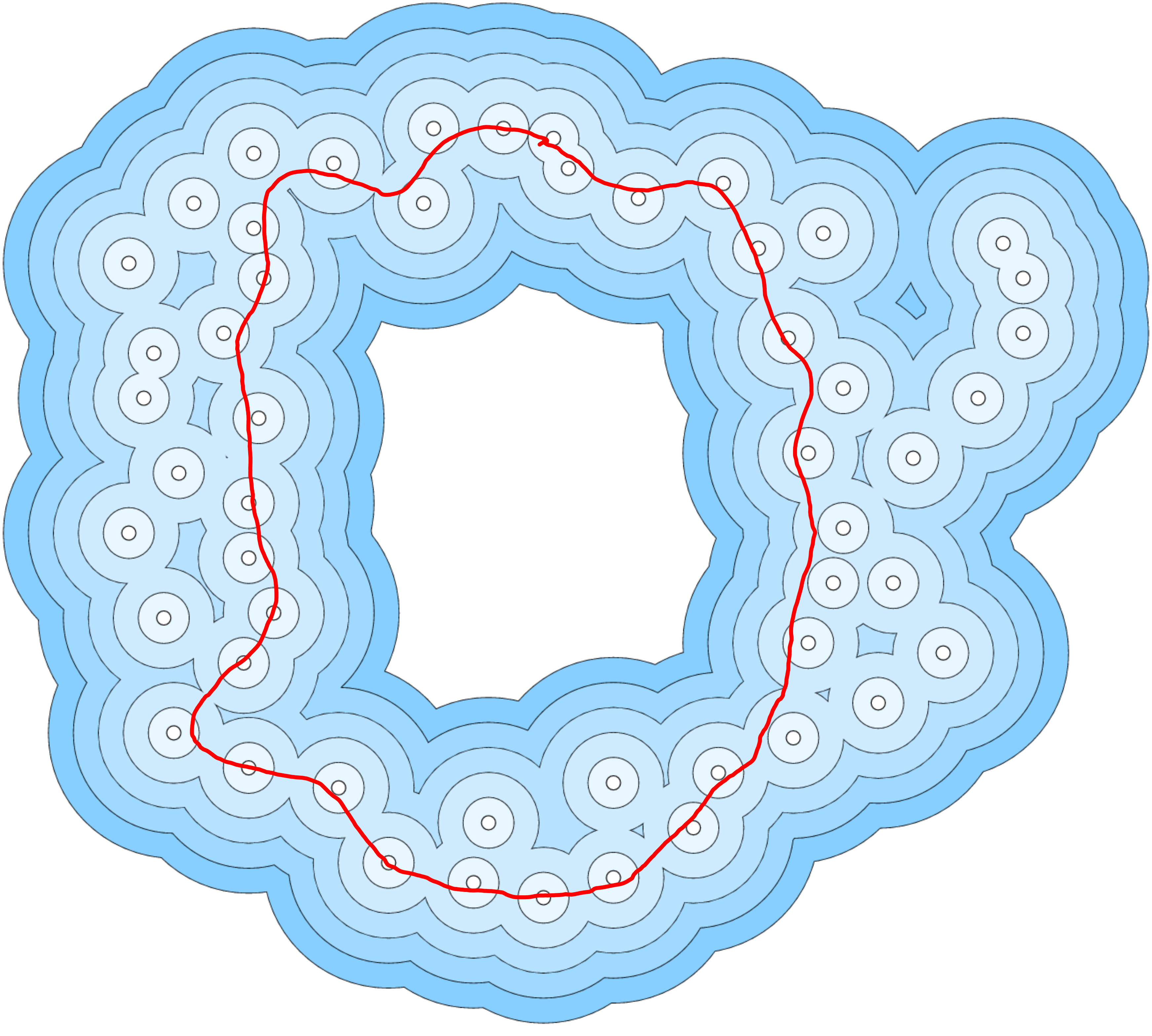


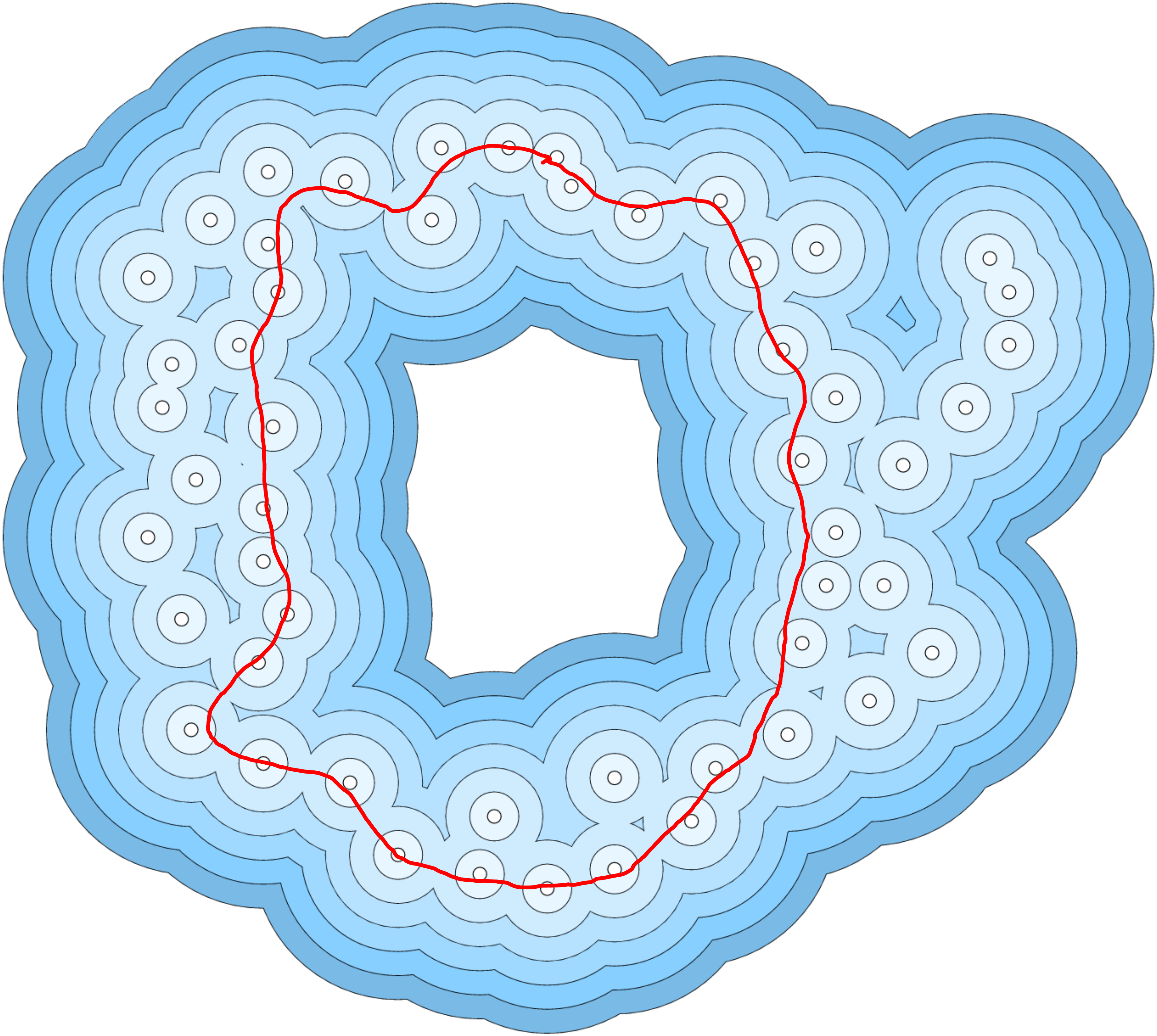


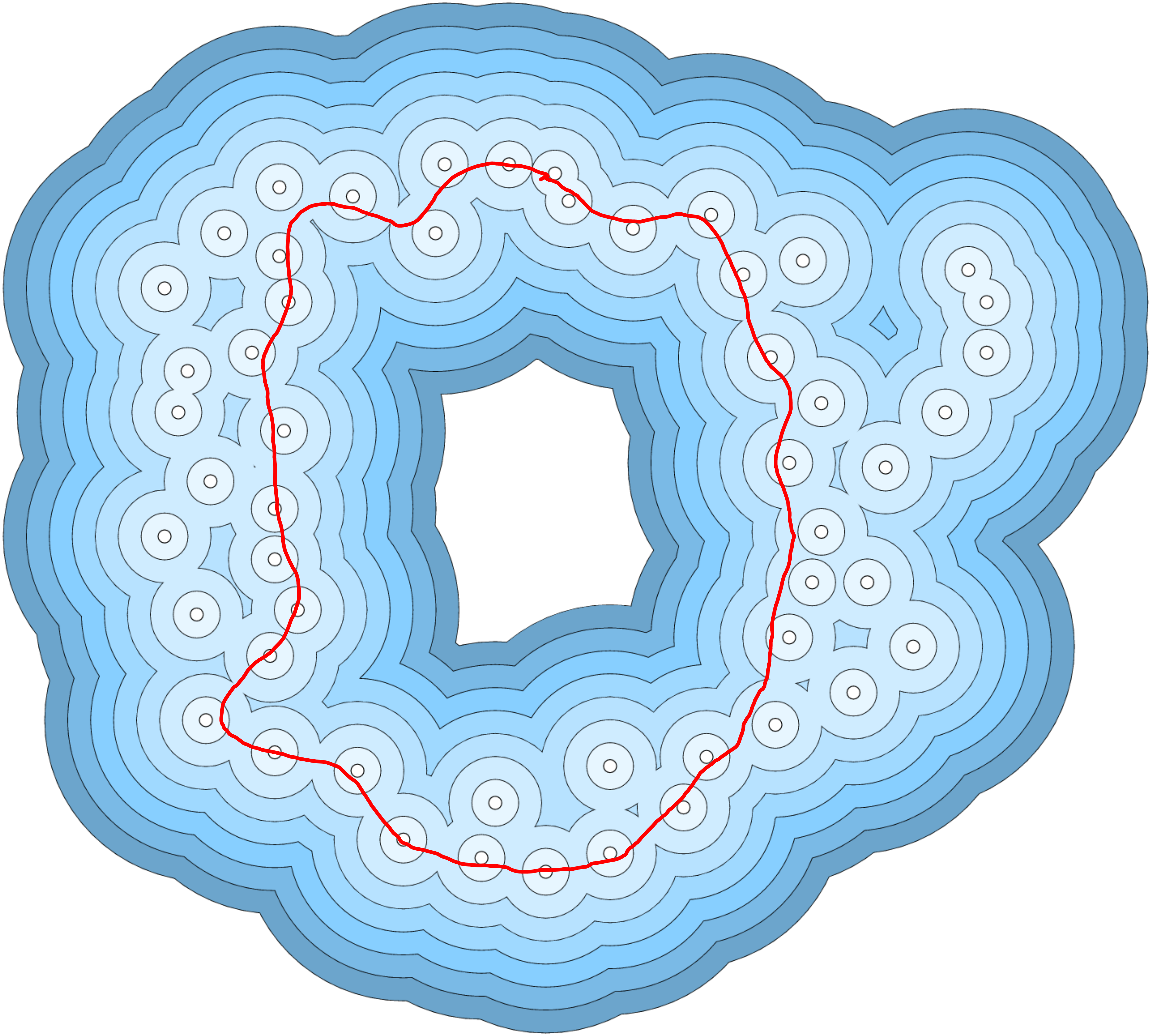


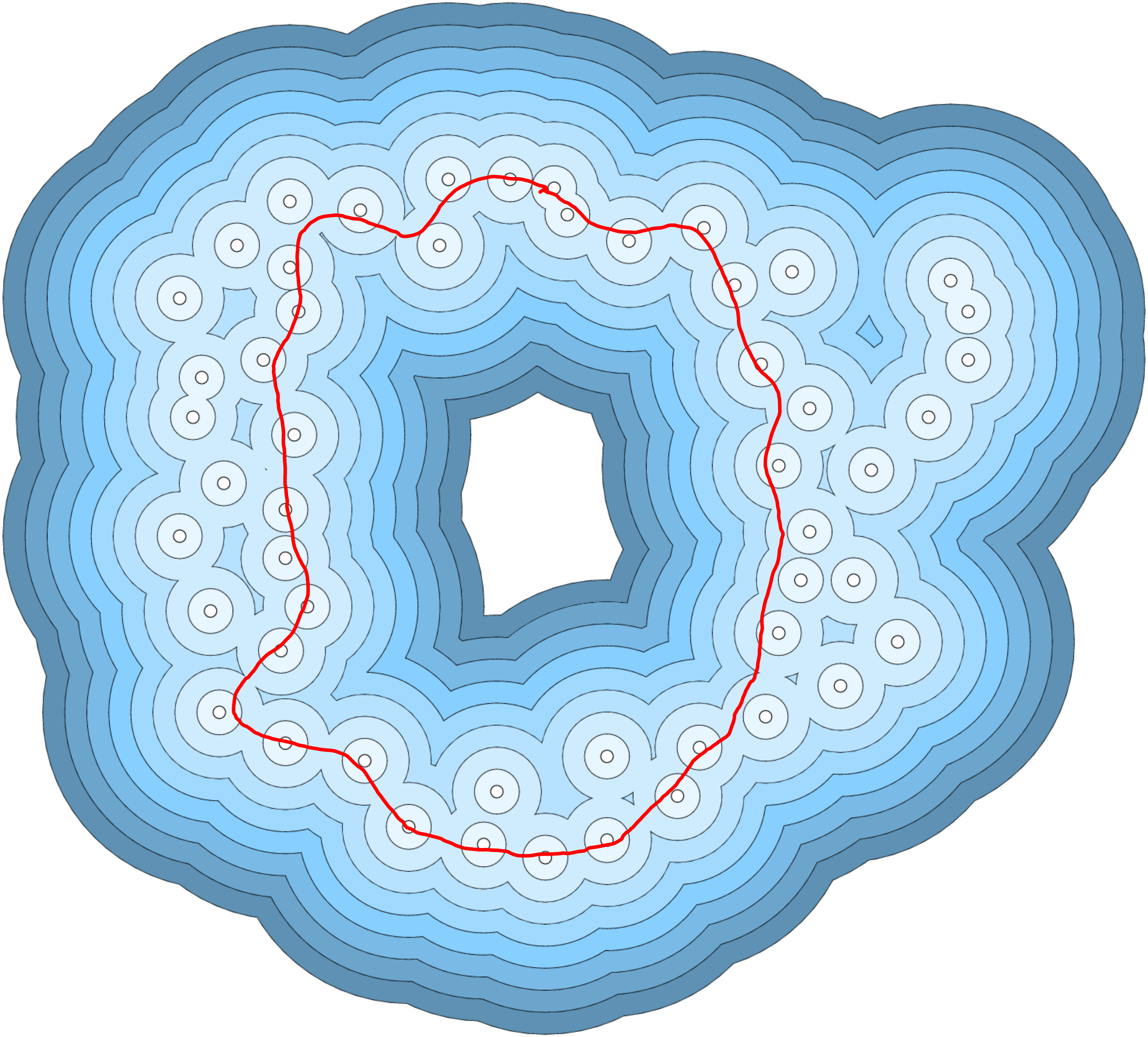




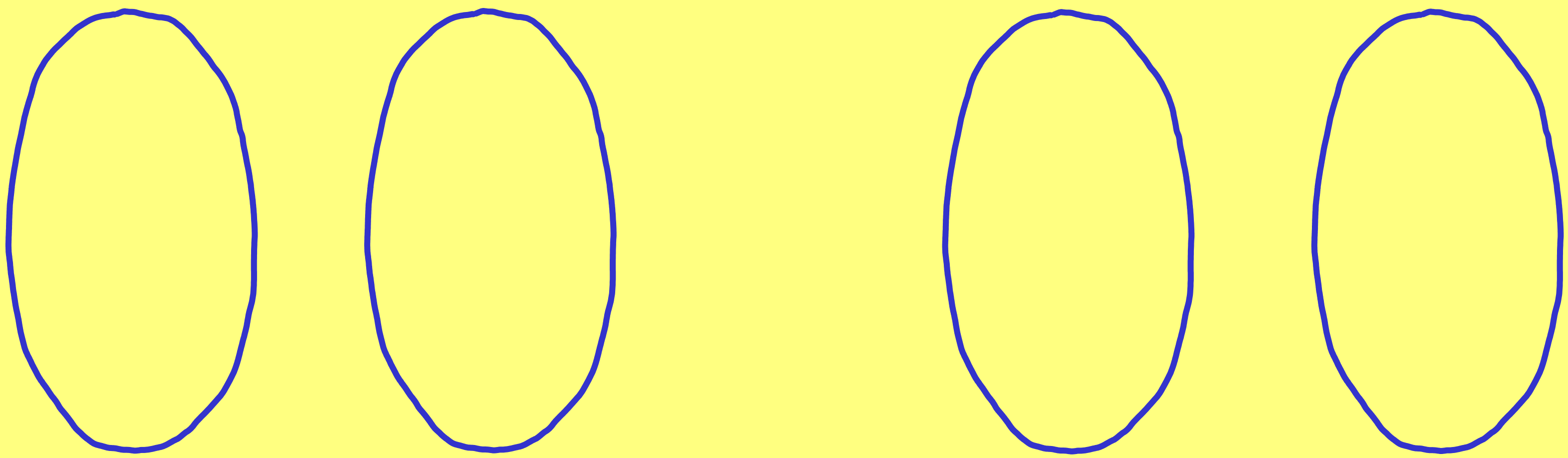






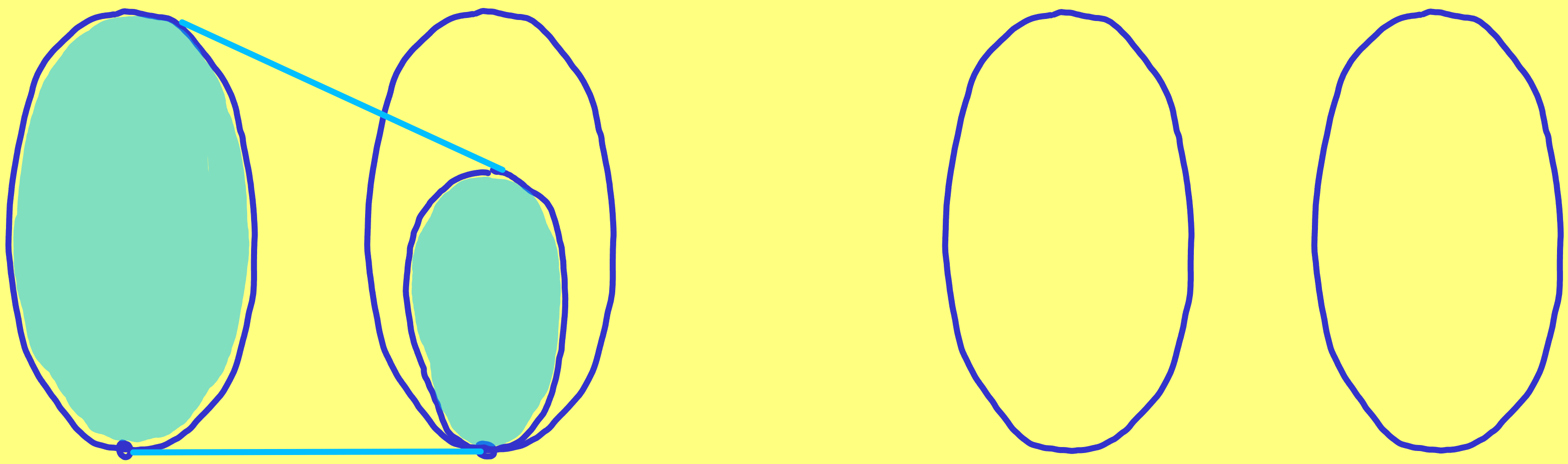


Persistence



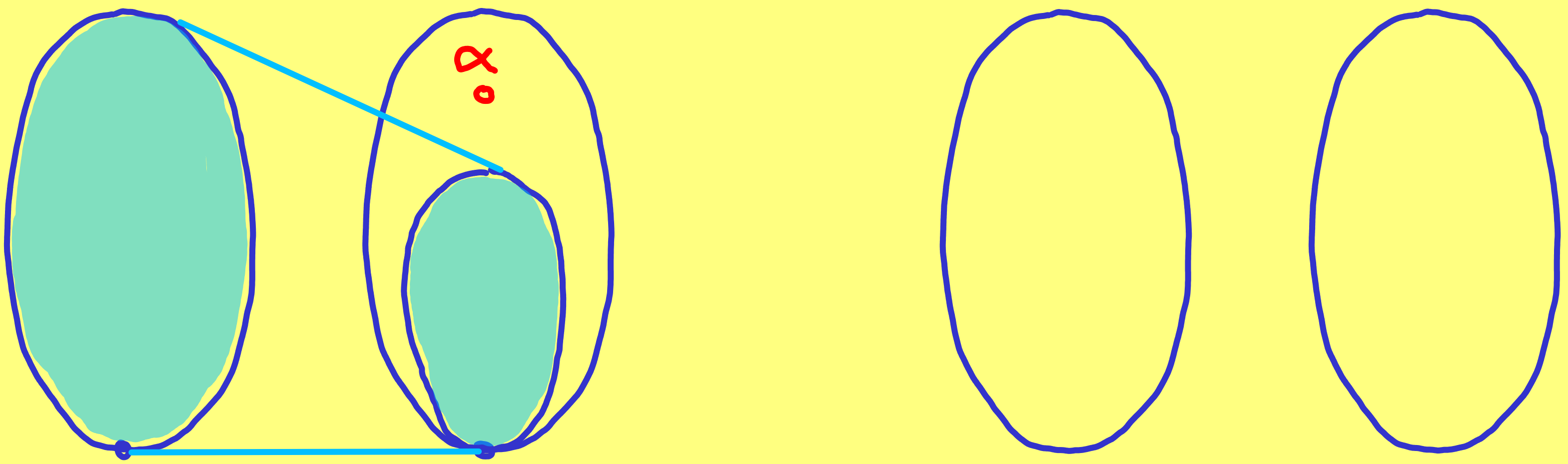
$$\dots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \dots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \dots$$

PERSISTENCE



$$\cdots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \cdots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \cdots$$

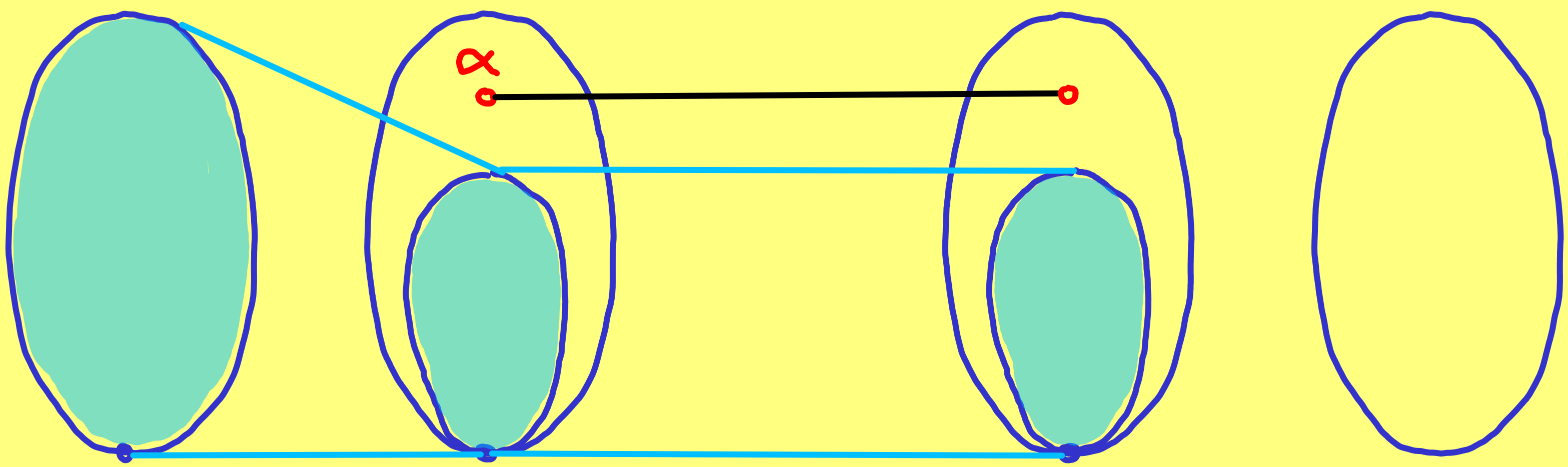
Persistence



$$\dots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \dots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \dots$$

α is born at $\mathbb{X}_i$

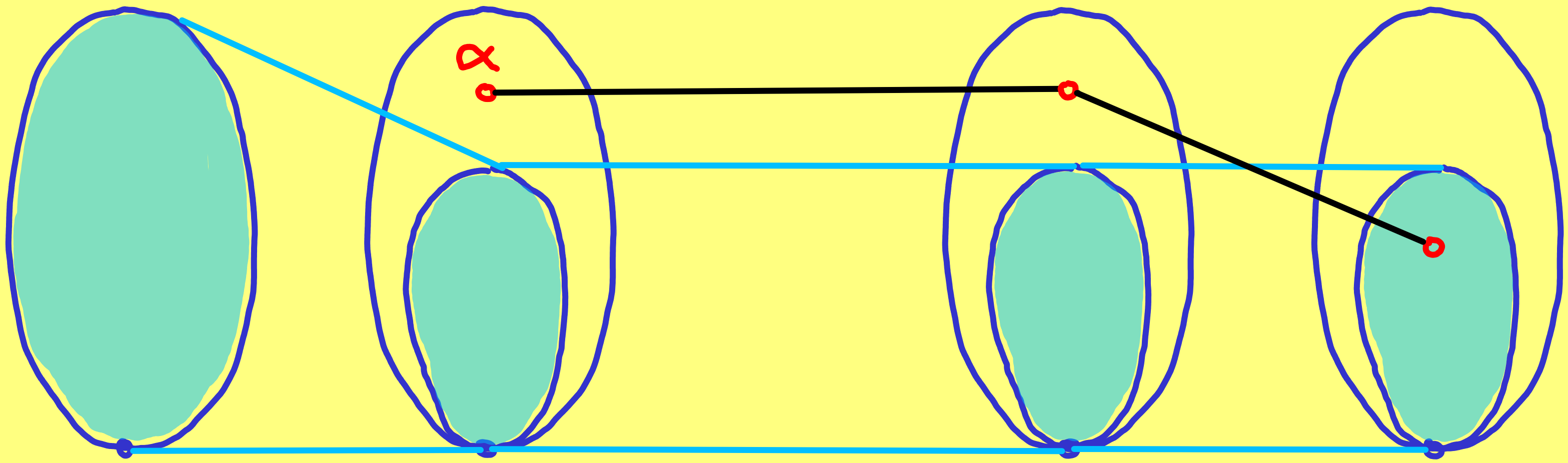
PERSISTENCE



$$\dots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \dots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \dots$$

α is born at $\mathbb{X}_i$

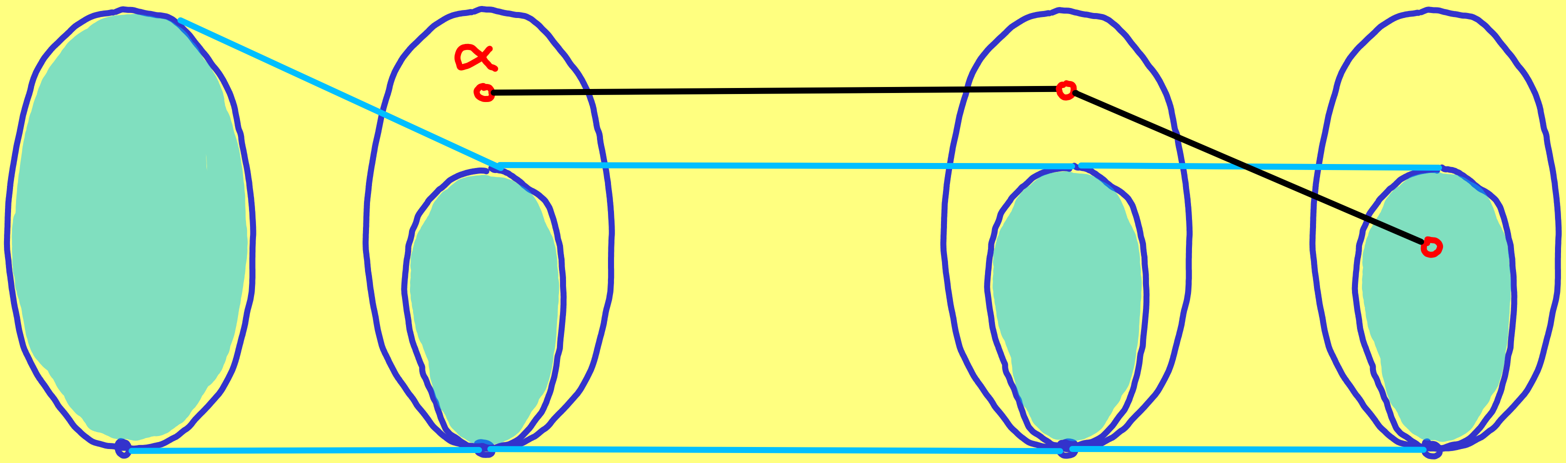
Persistence



$$\cdots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \cdots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \cdots$$

α is born at $\mathbb{X}_i$ and dies entering $\mathbb{X}_j$

PERSISTENCE

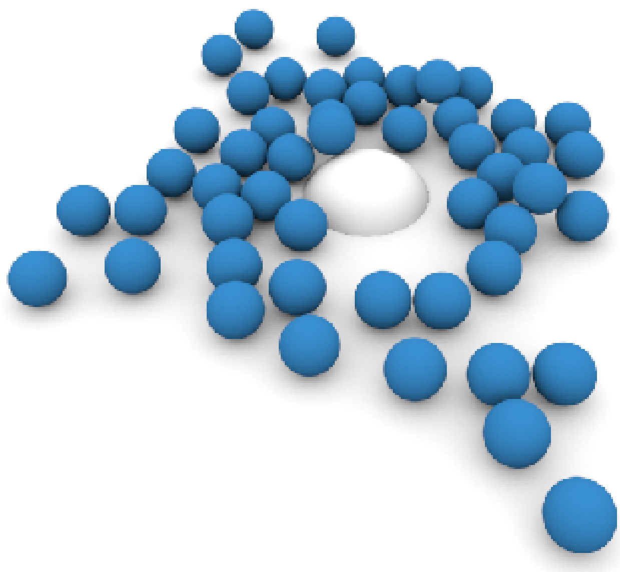


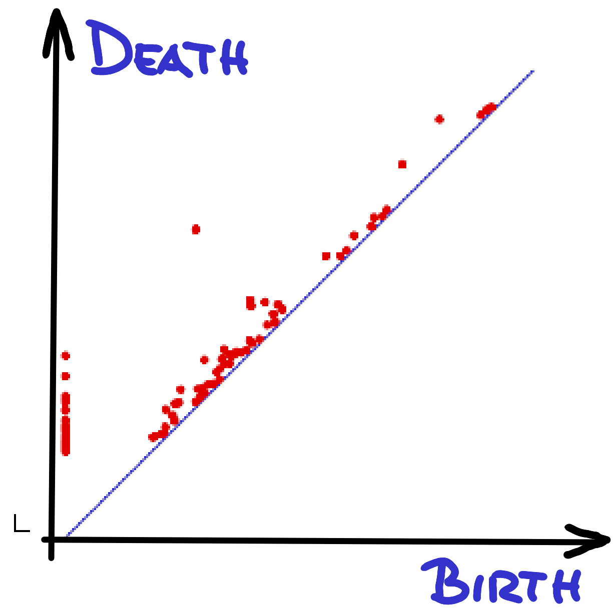
$$\dots \to H(\mathbb{X}_{i-1}) \to H(\mathbb{X}_i) \to \dots \to H(\mathbb{X}_{j-1}) \to H(\mathbb{X}_j) \to \dots$$

α is born at $\mathbb{X}_i$ and dies entering $\mathbb{X}_j$

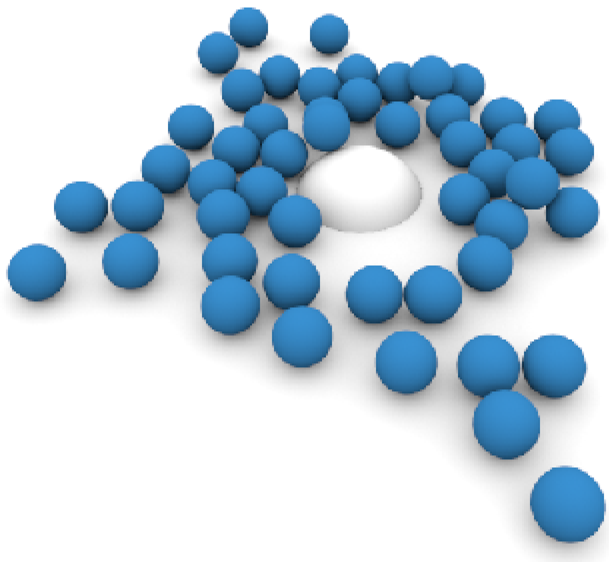
[E., Letscher, Zomorodian 2000]

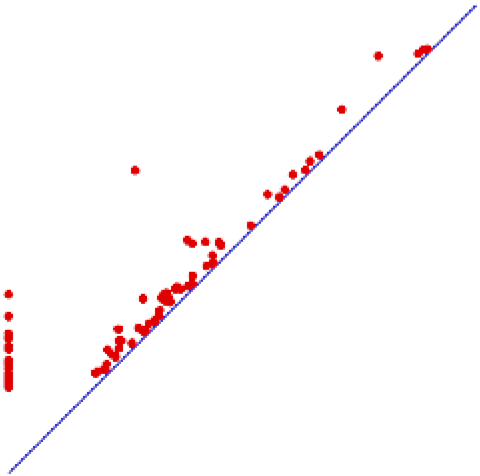
Stability of persistence.



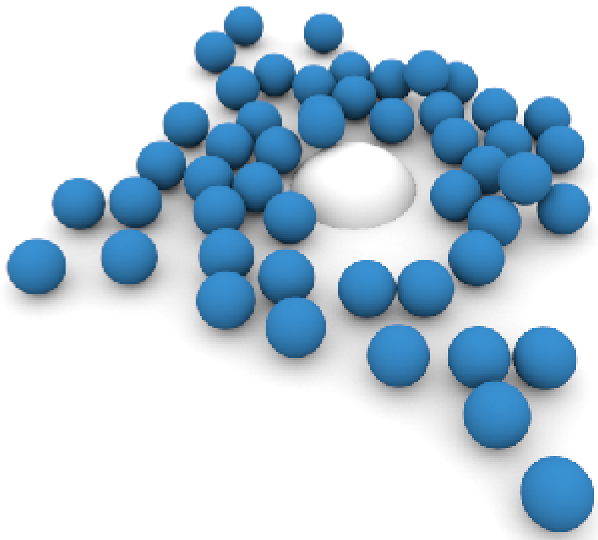


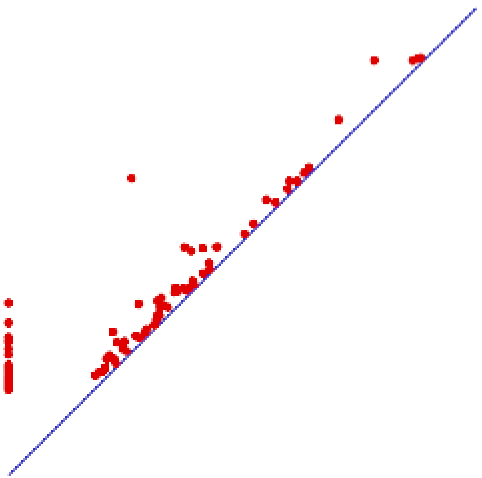
Stability of persistence.





Stability of persistence.





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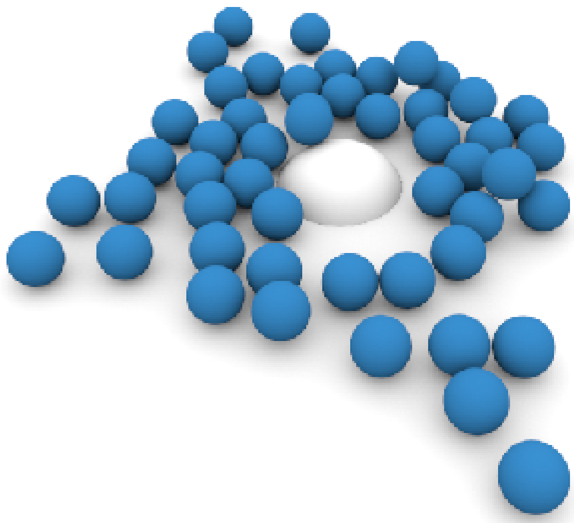

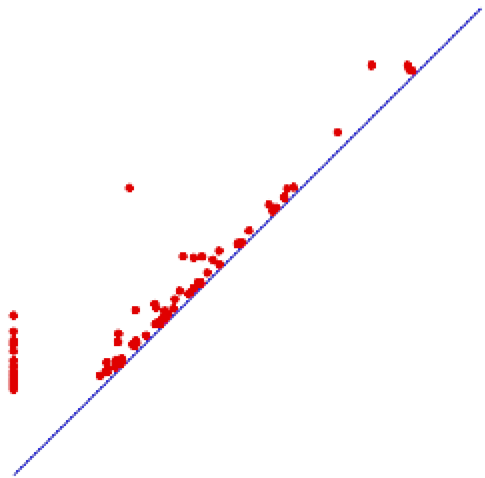

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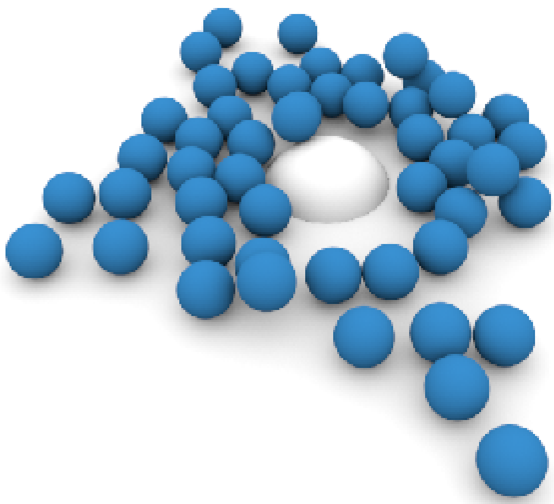

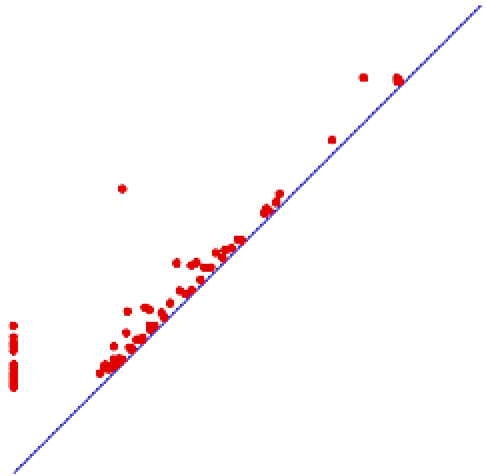

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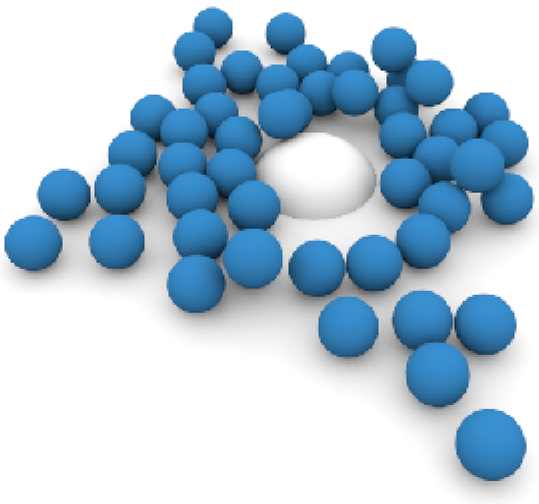

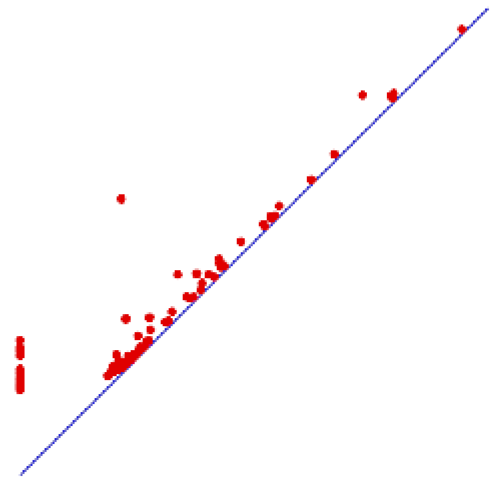

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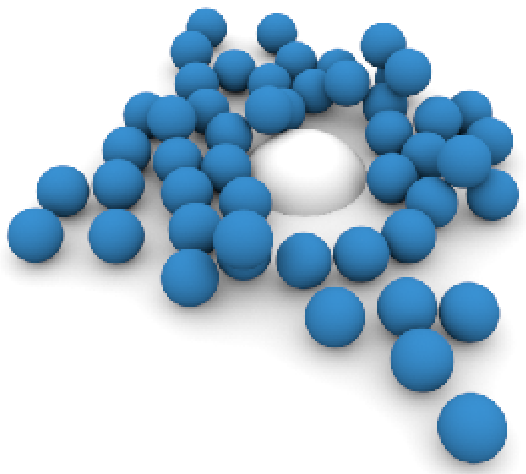

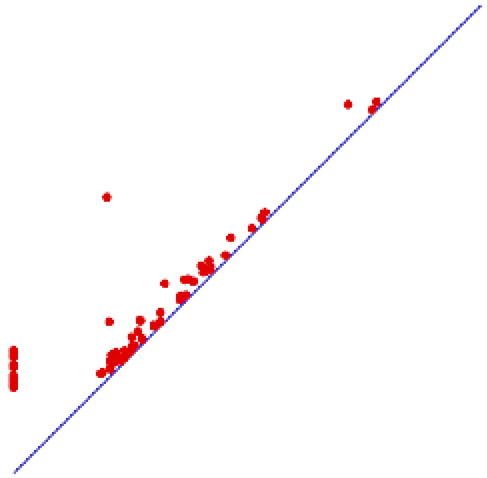

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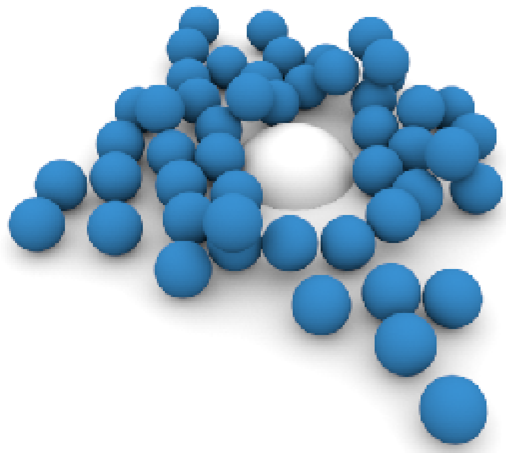

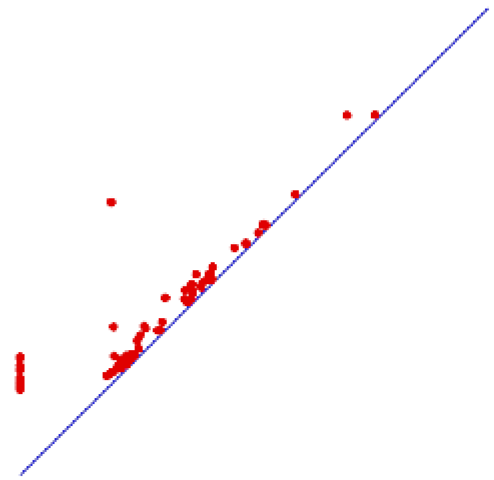

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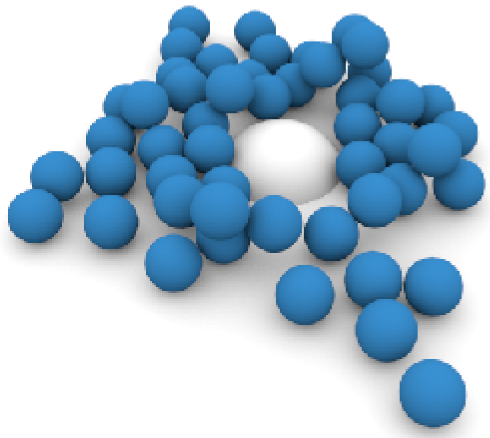

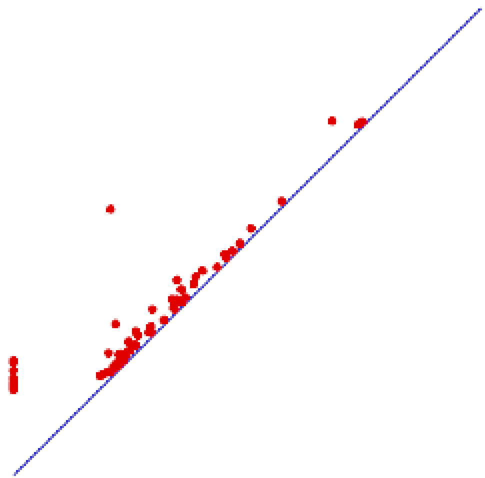

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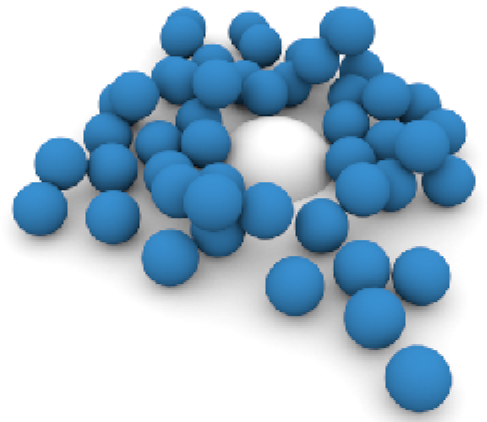

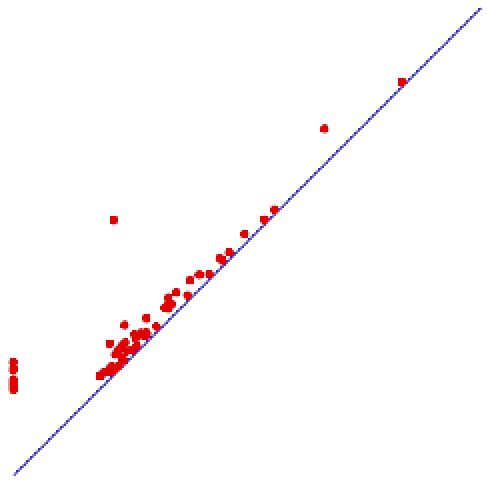

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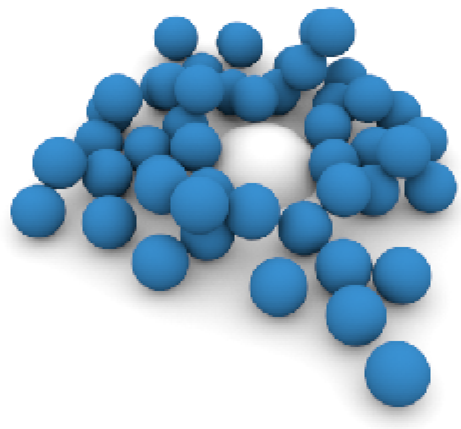

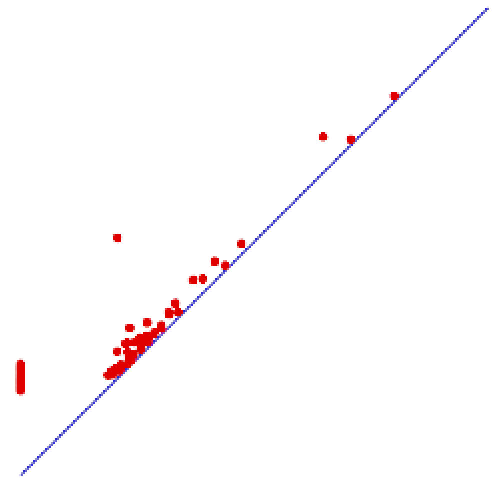

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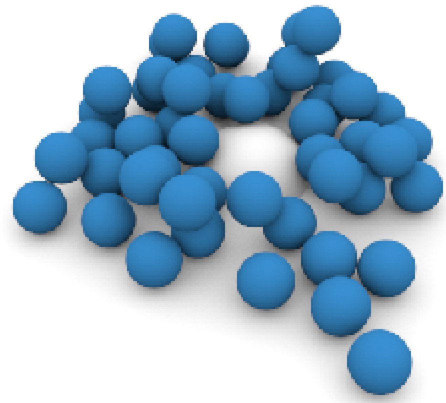

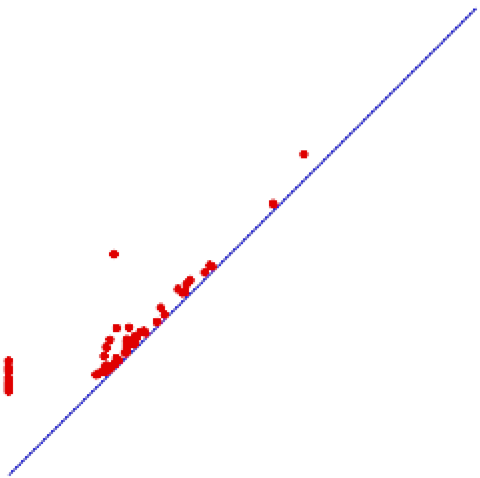

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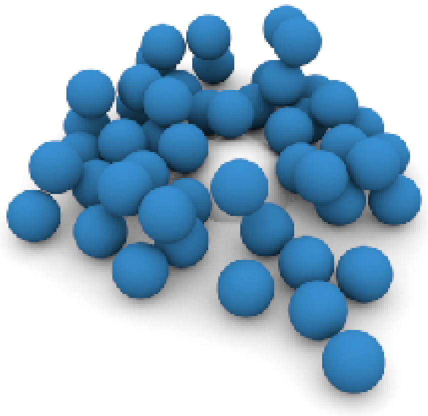

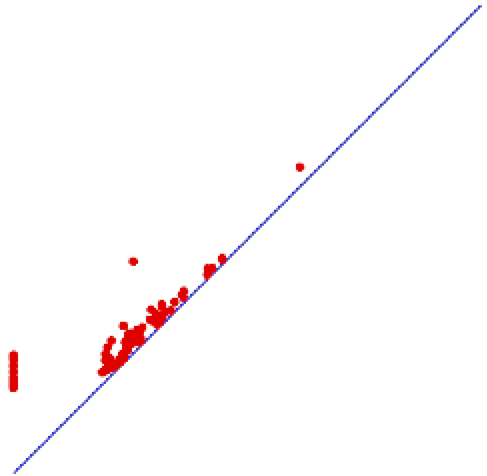

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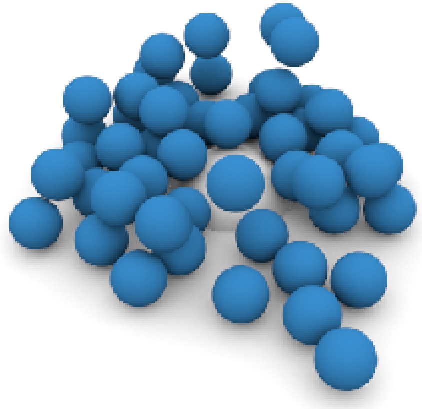

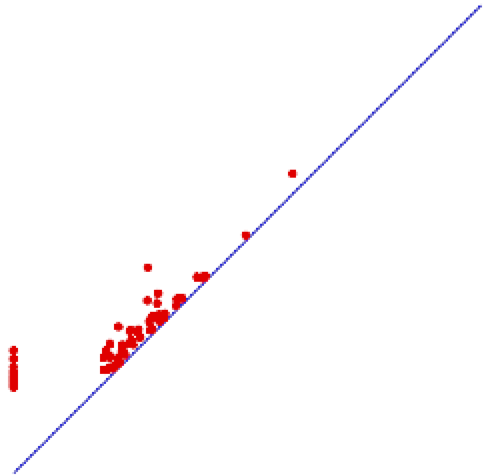

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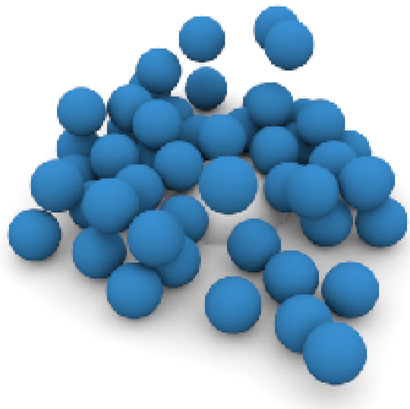

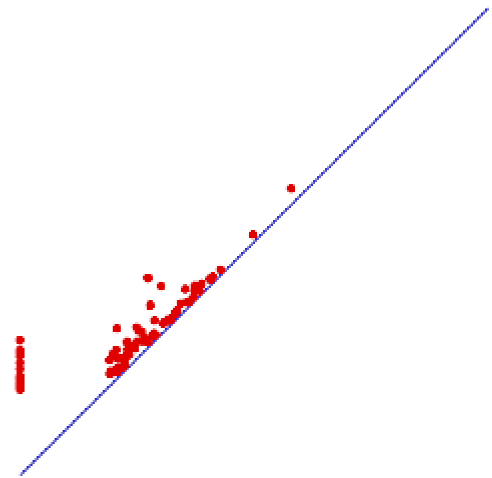

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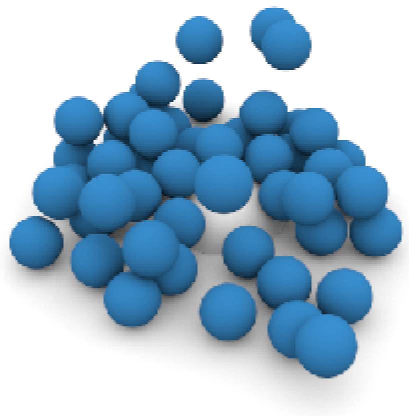

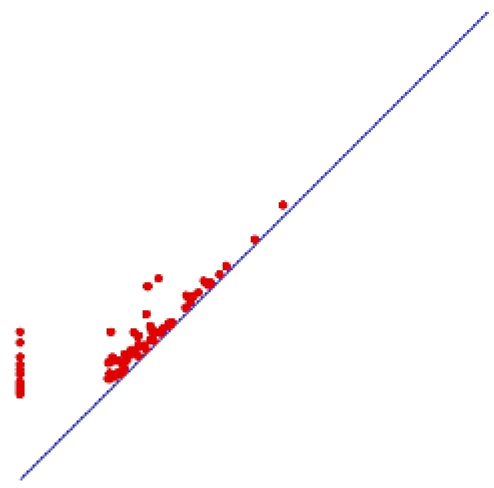

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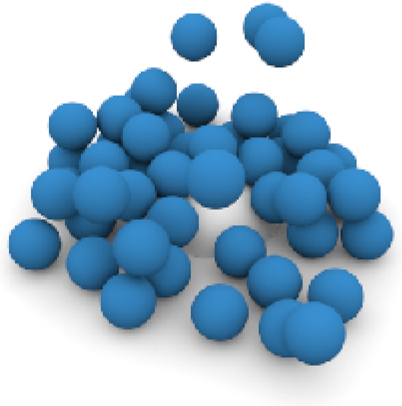

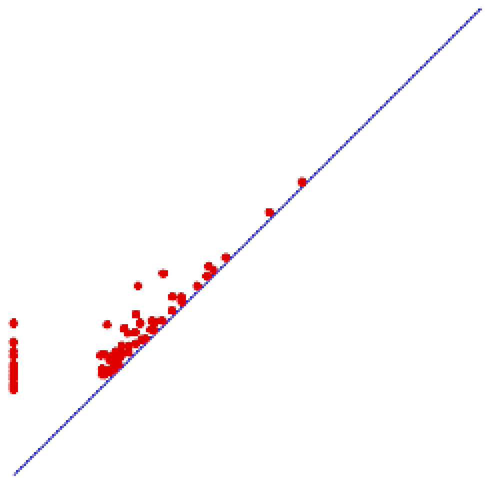

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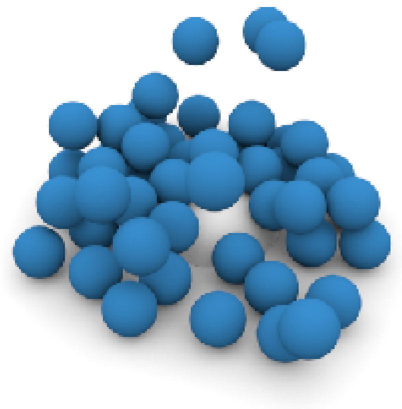

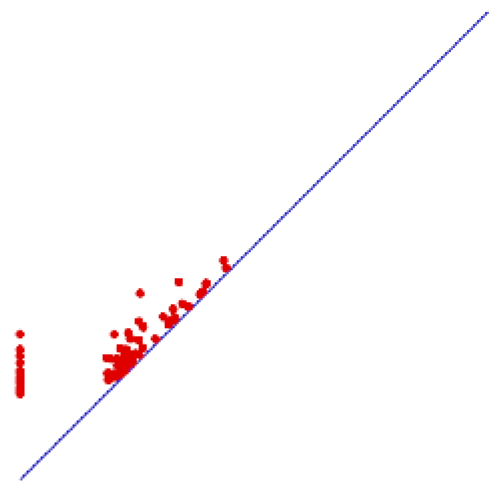

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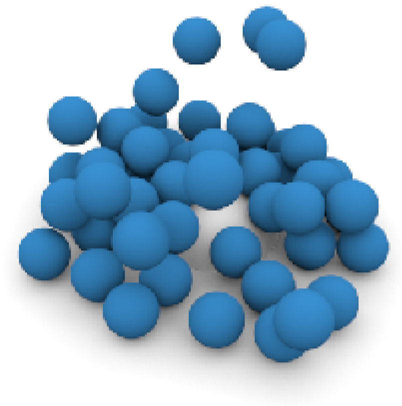

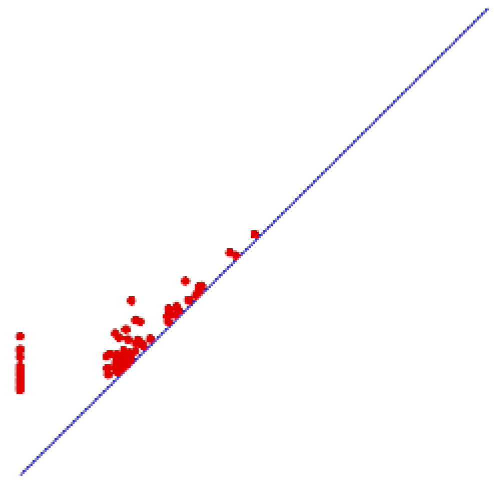

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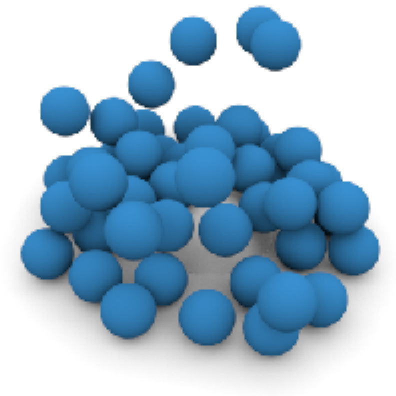

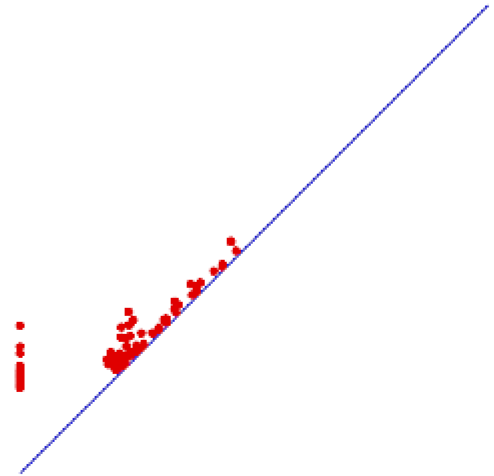

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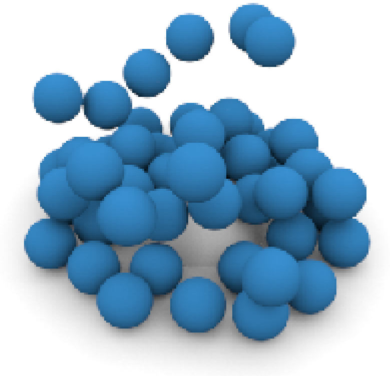

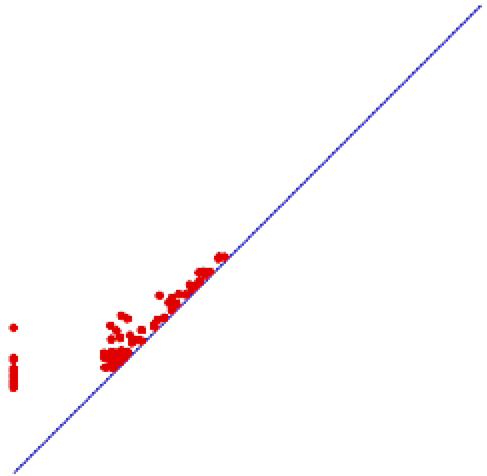

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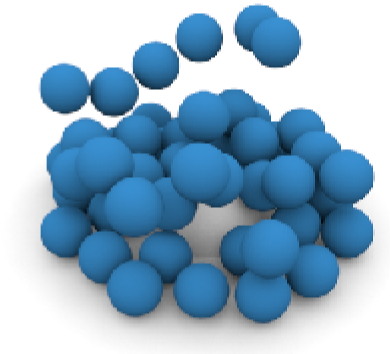

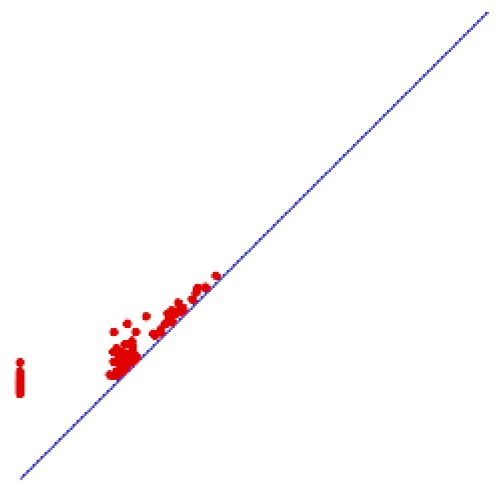

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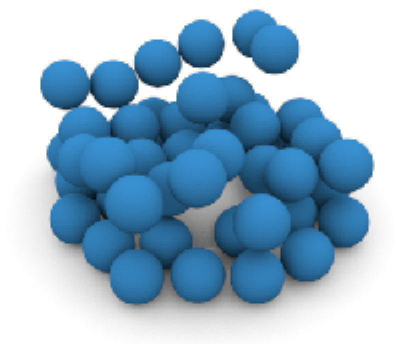

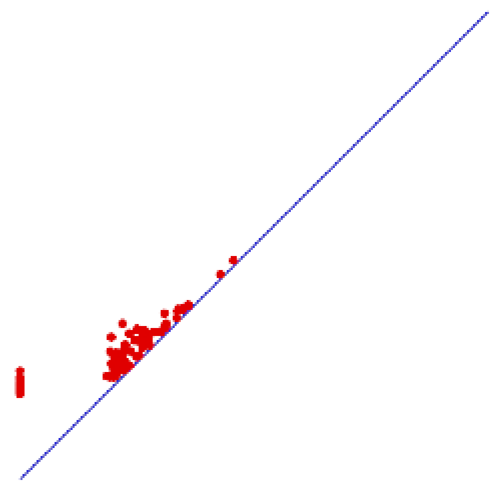

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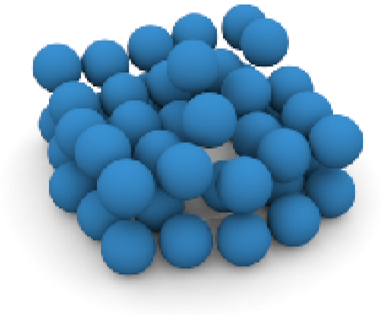

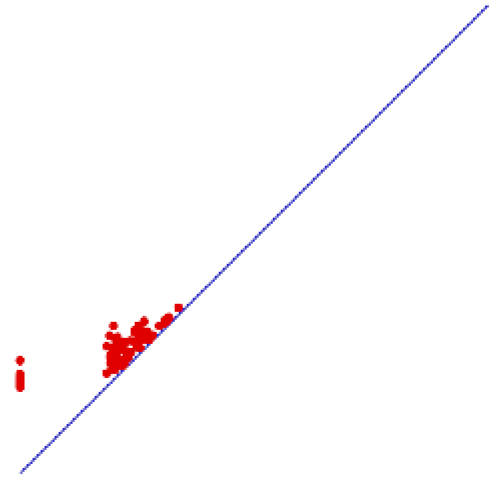

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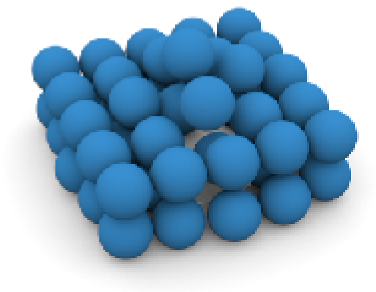

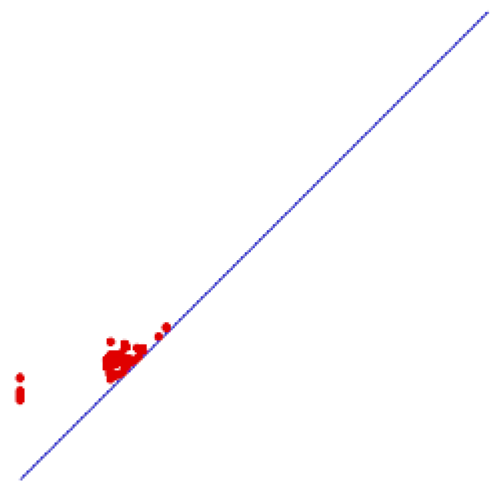

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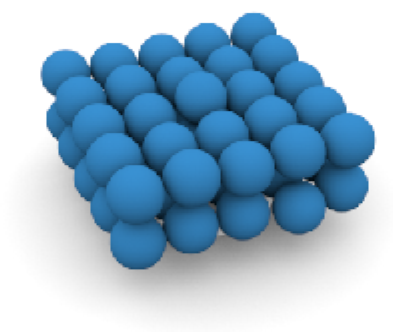

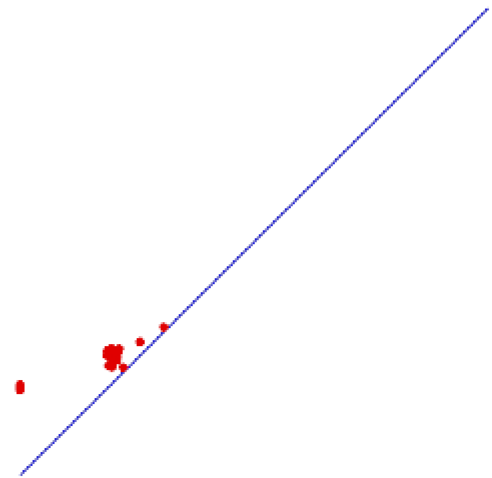

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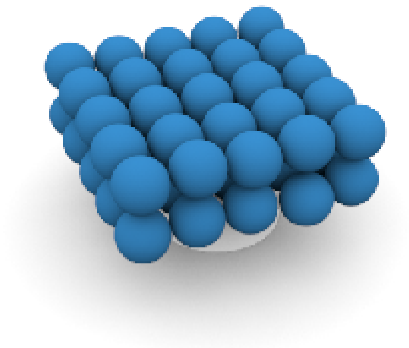

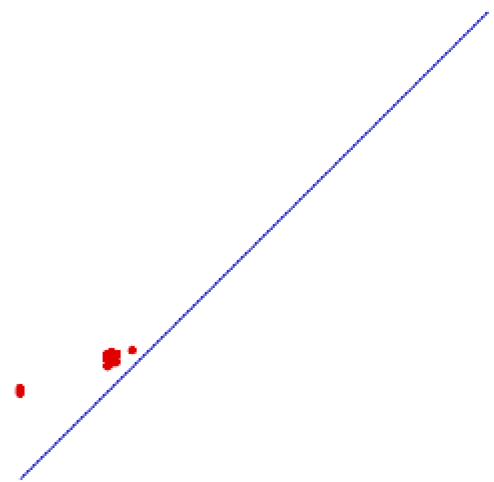

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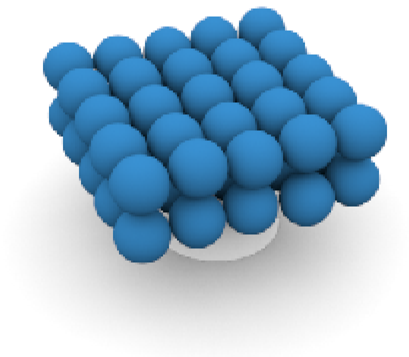

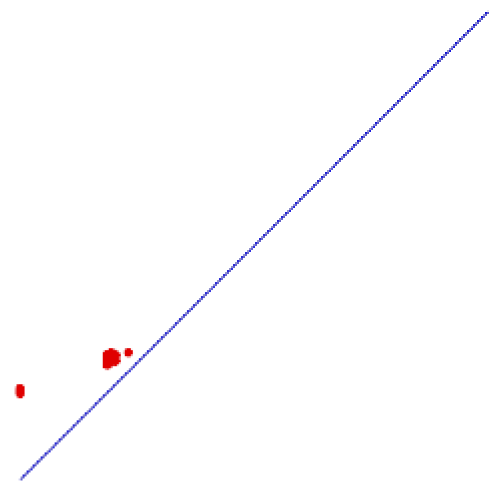

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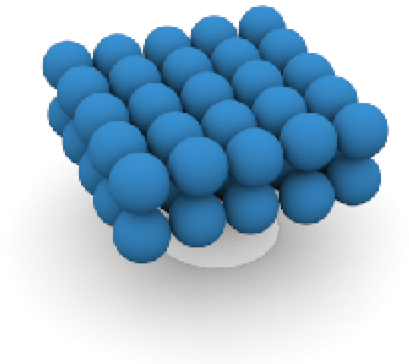
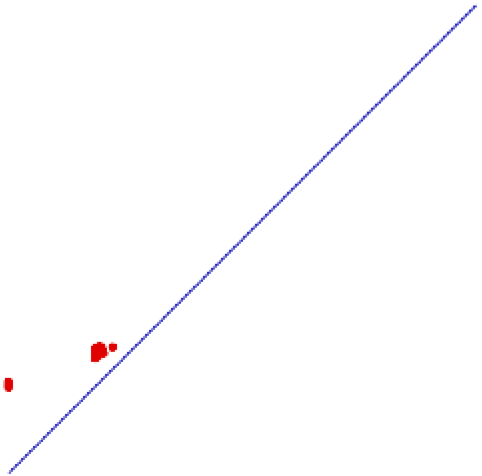
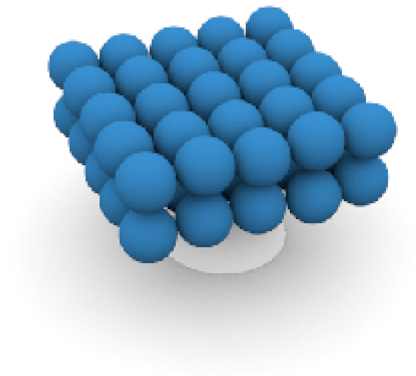
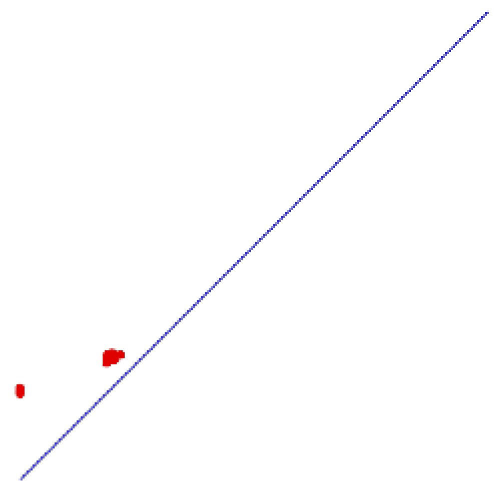


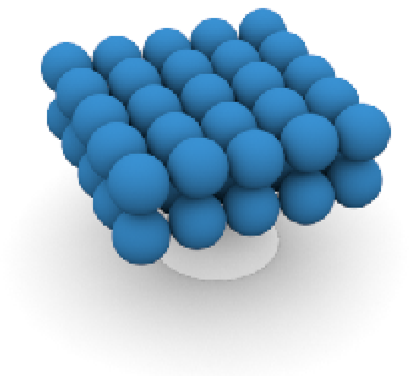


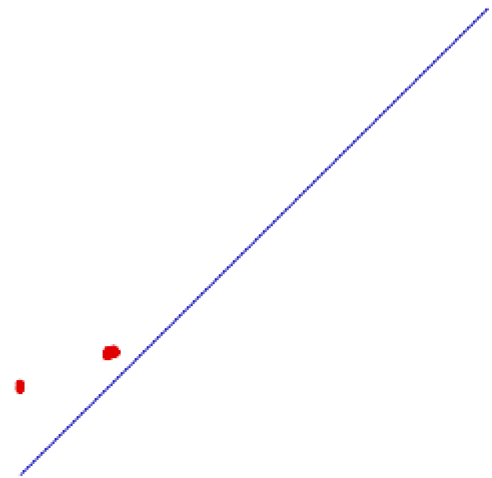
Stability of persistence.



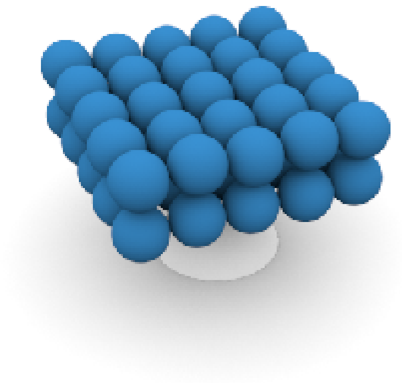


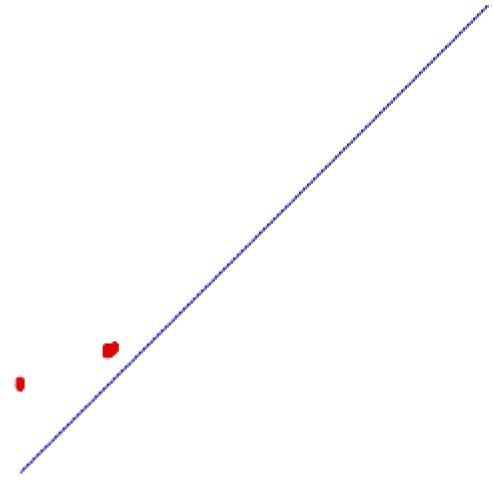
Stability of persistence.





Stability of persistence.





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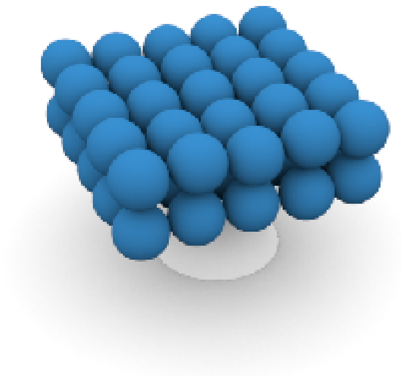

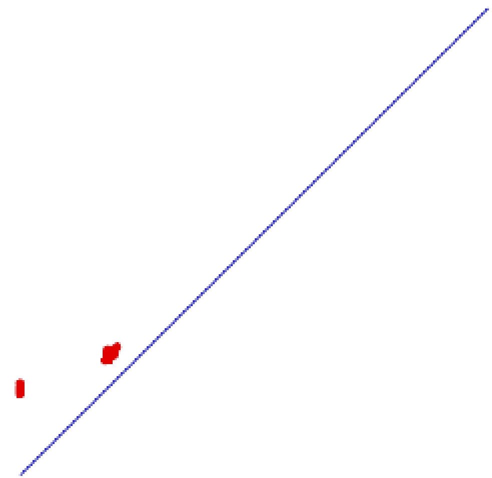

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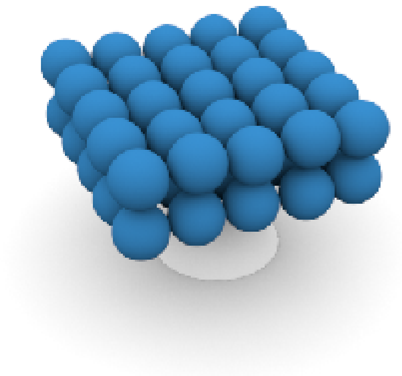

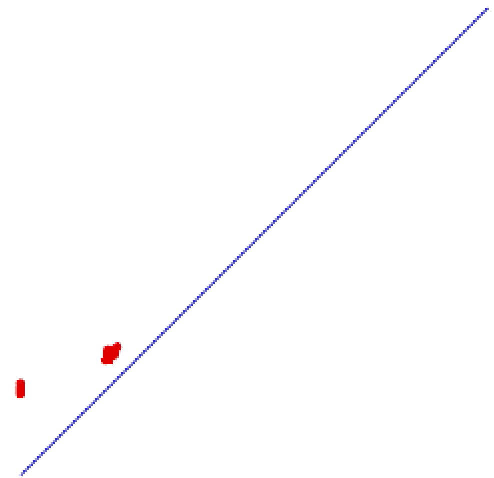

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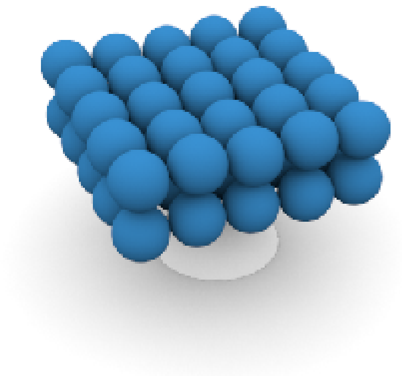

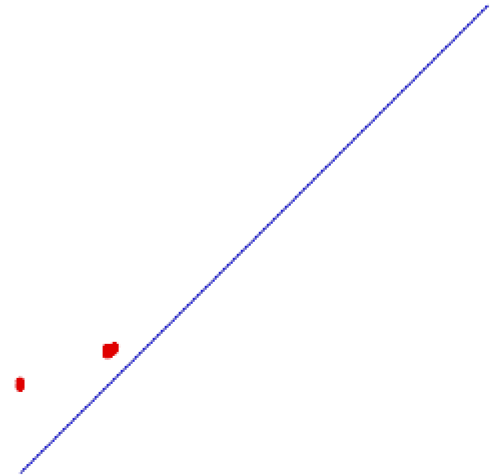

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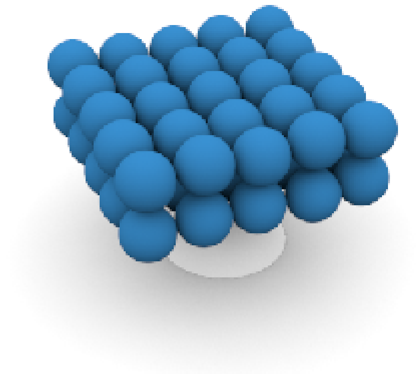

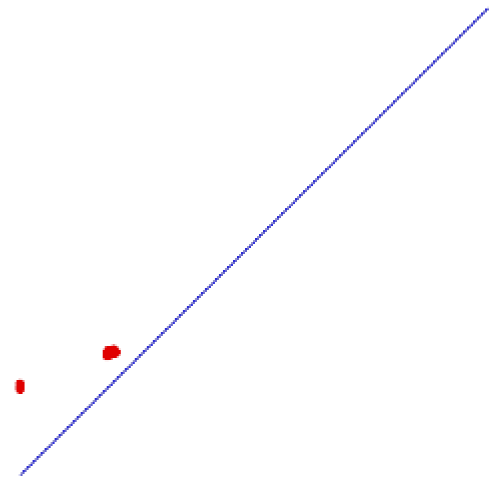

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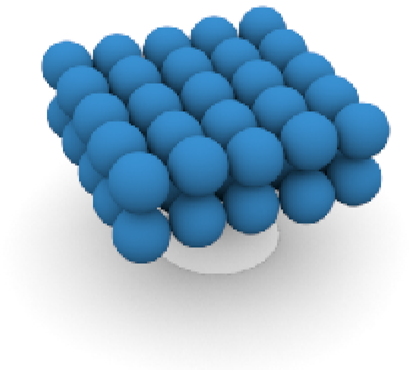

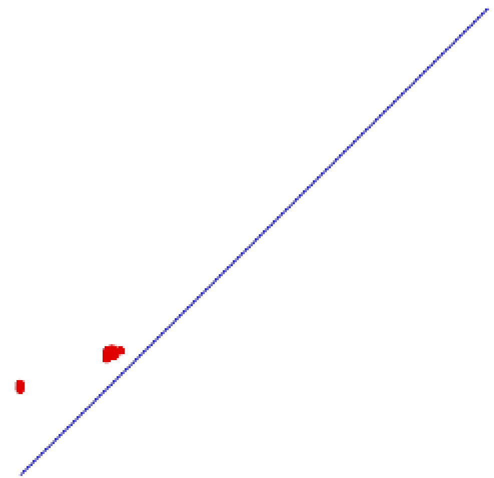

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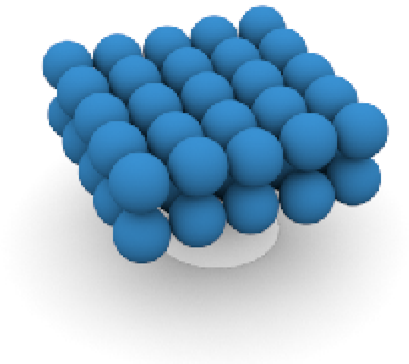

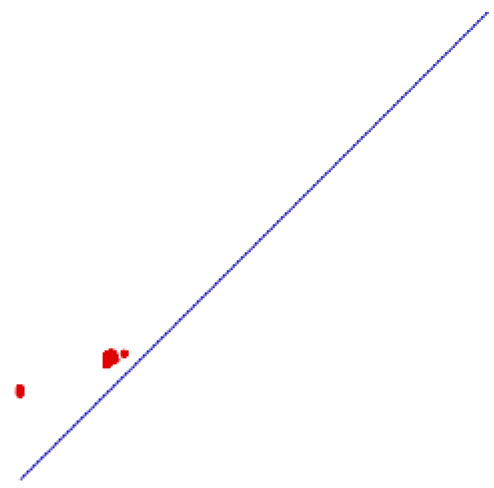

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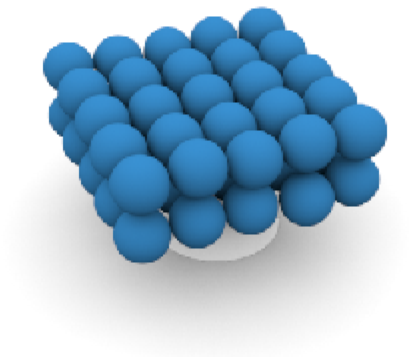

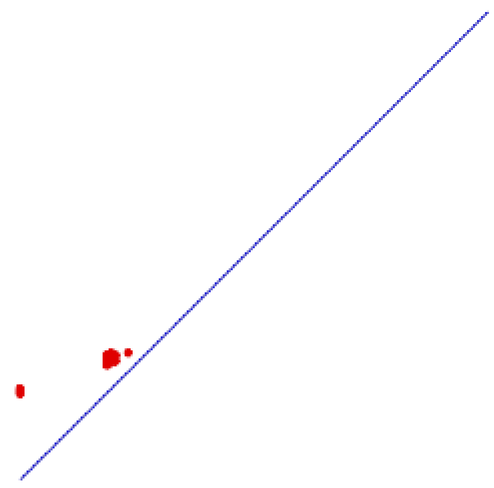

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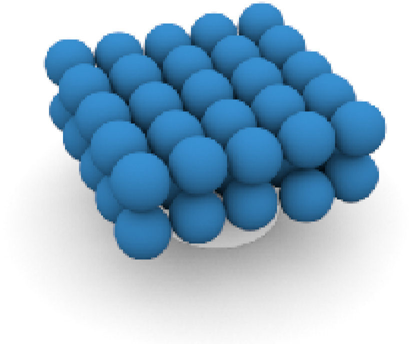

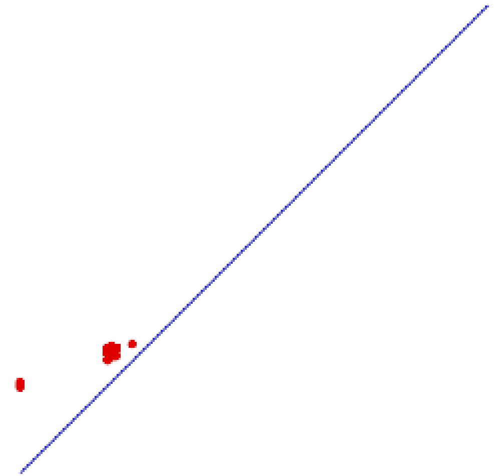

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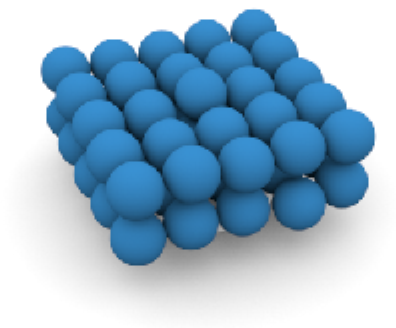

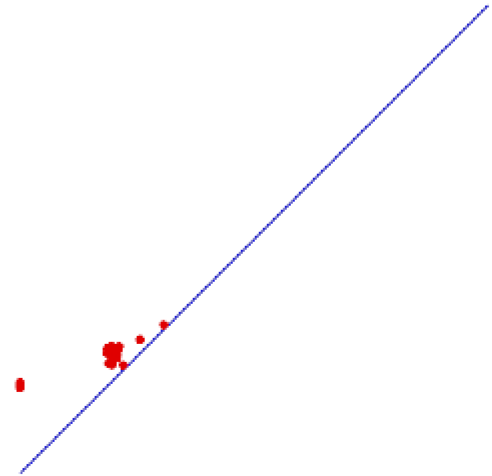

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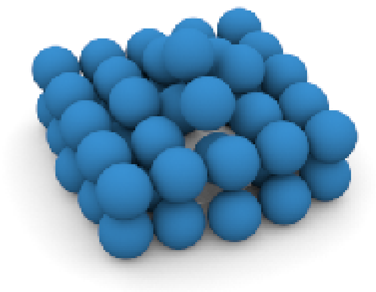

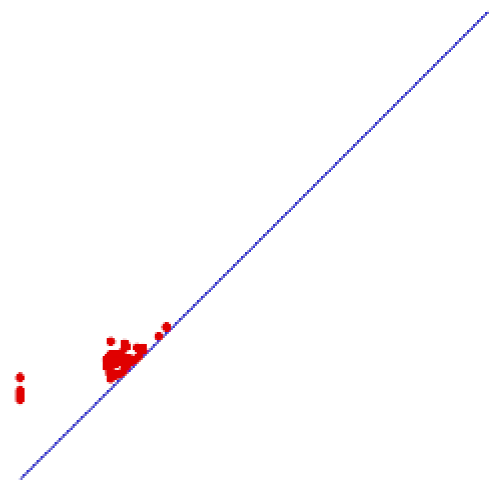

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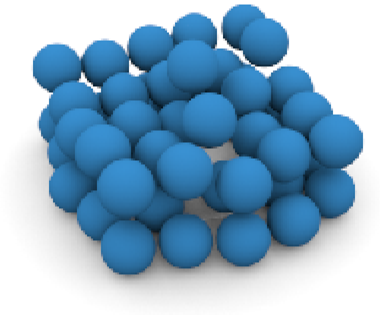

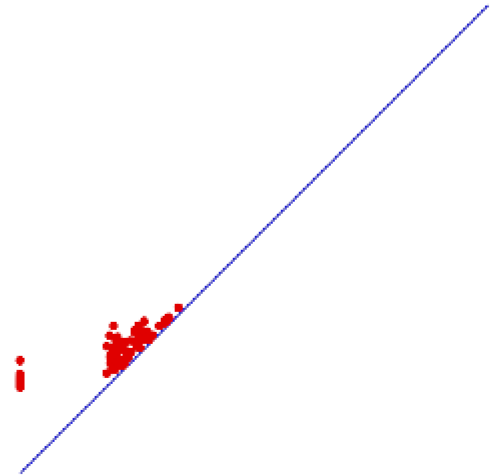

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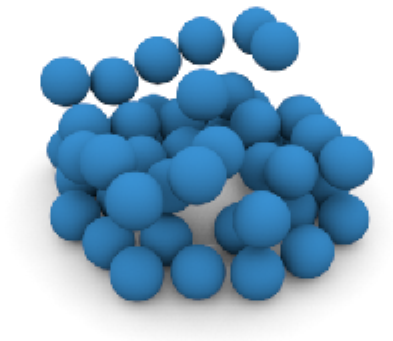

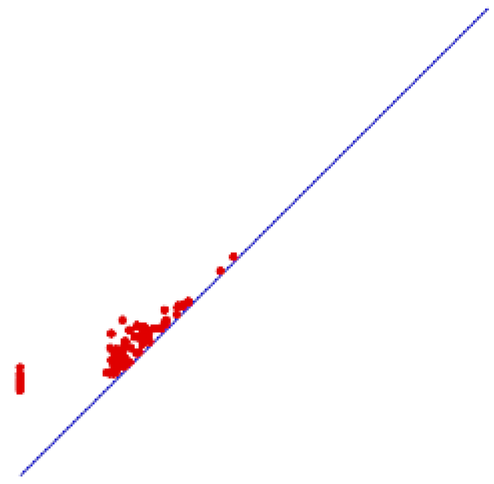

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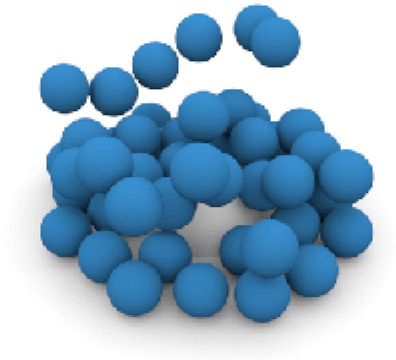

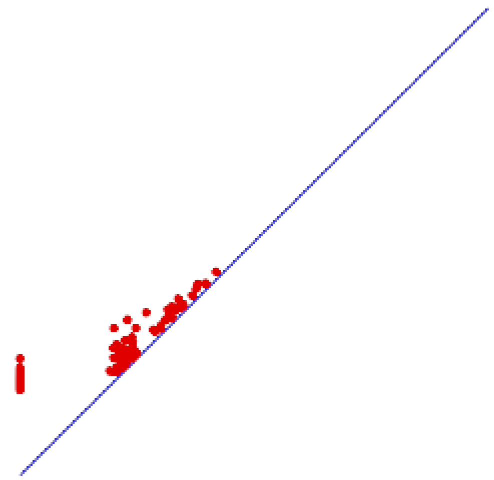

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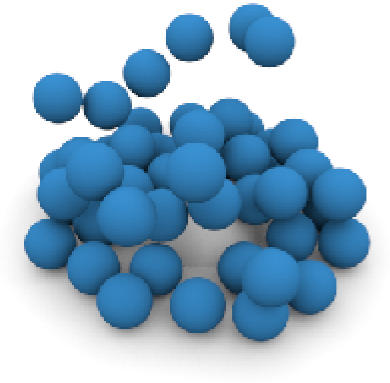

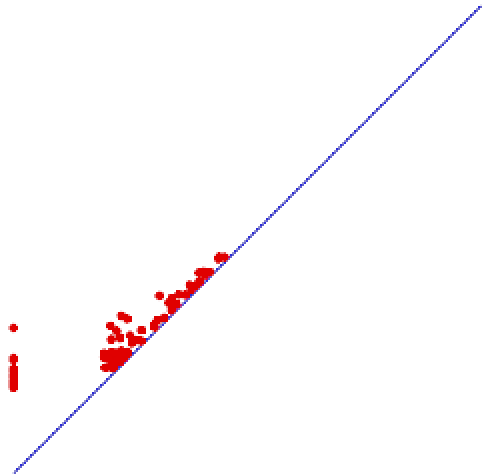

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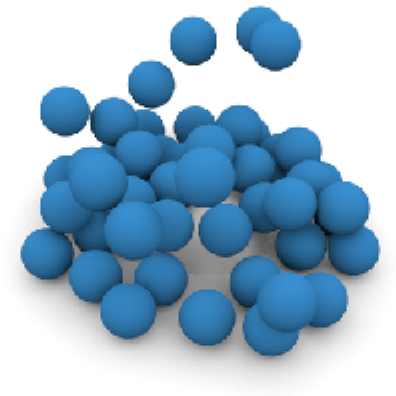

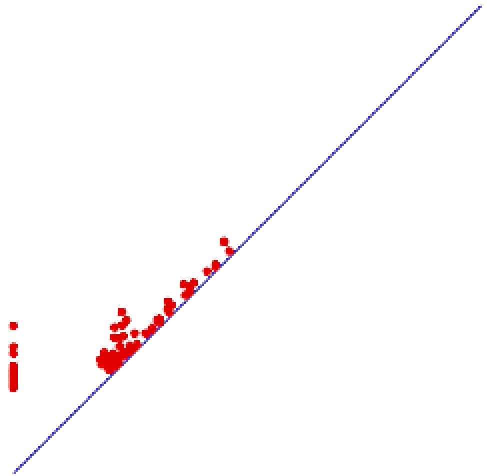

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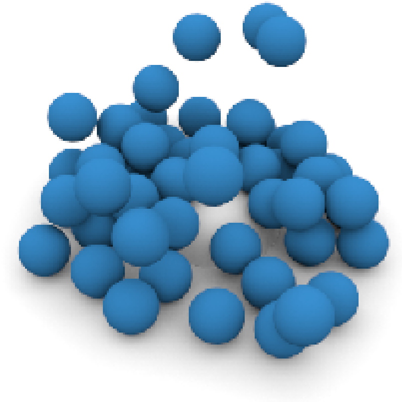

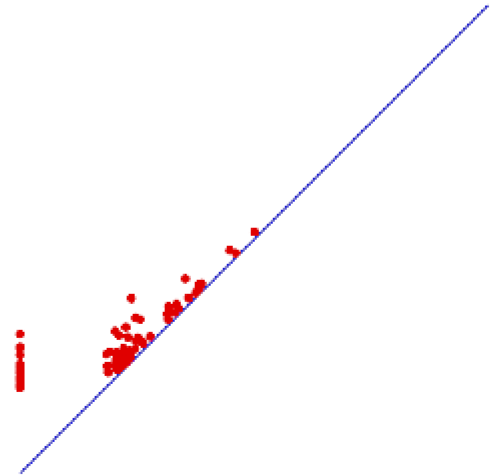

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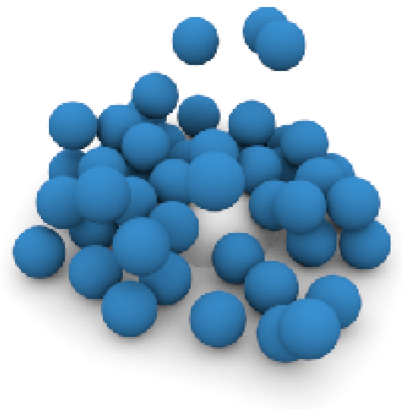

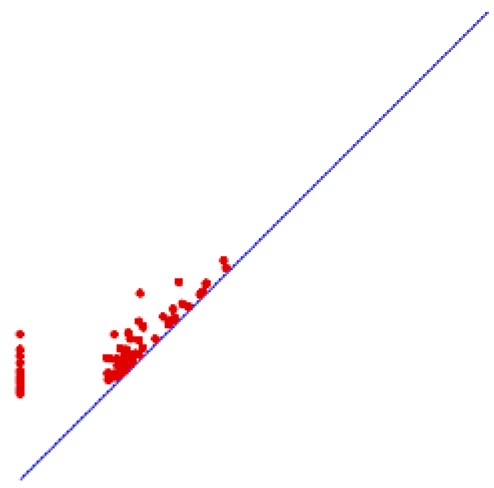

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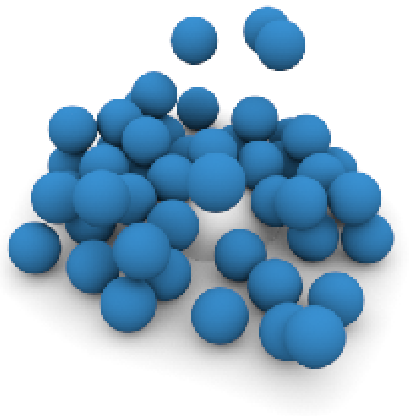

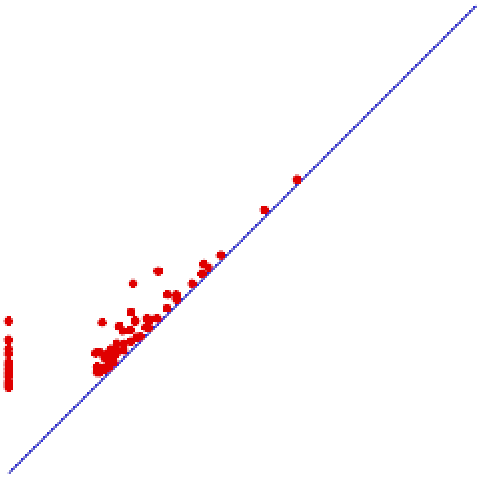

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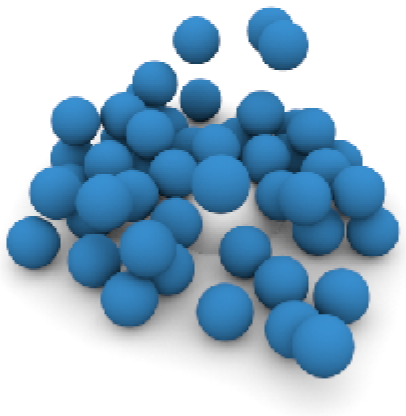

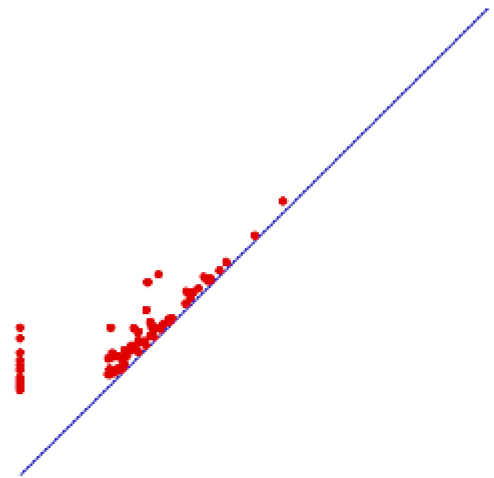

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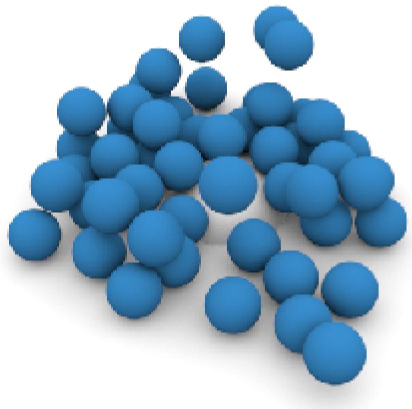

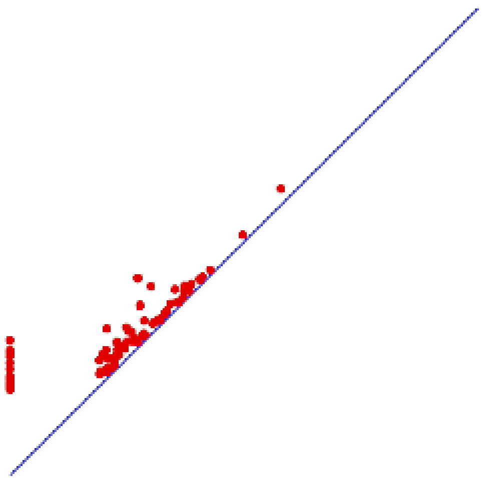

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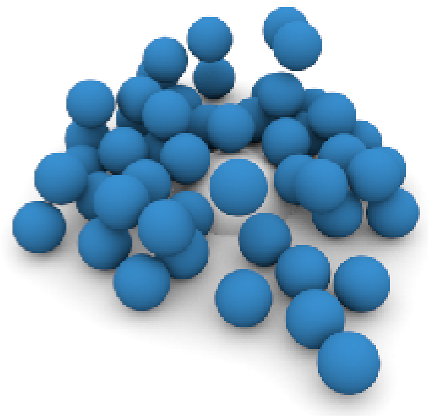

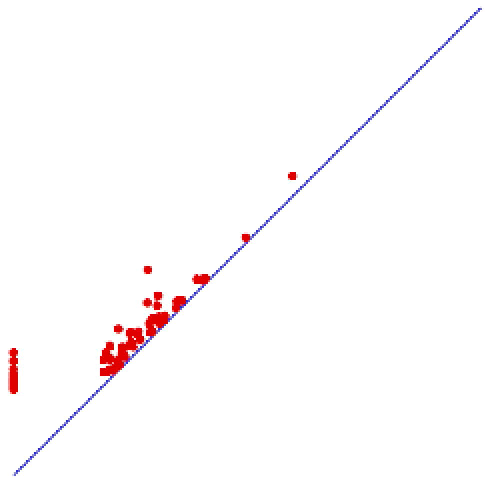

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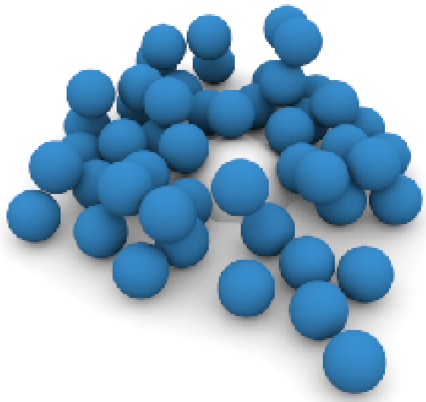

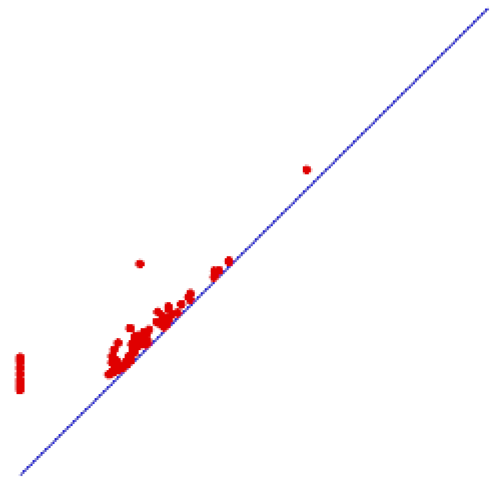

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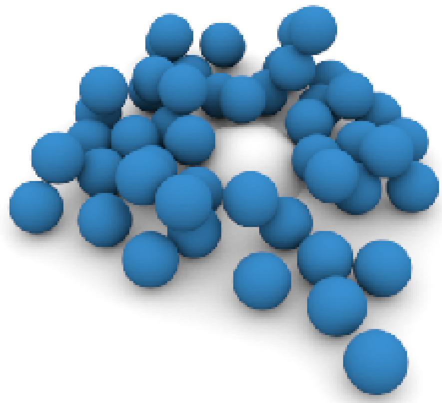

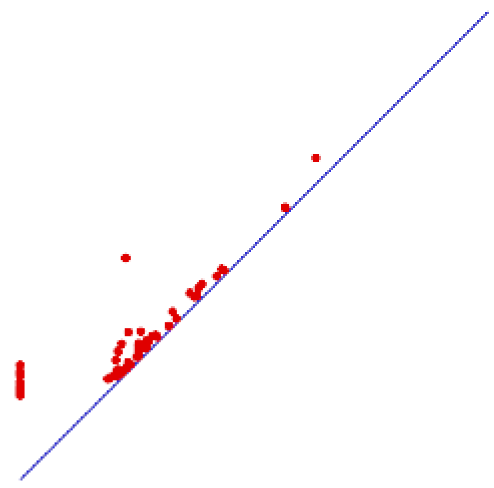

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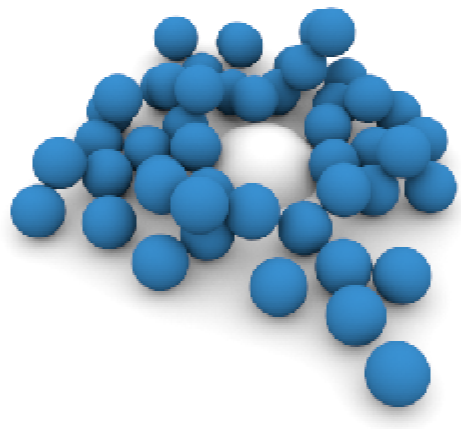

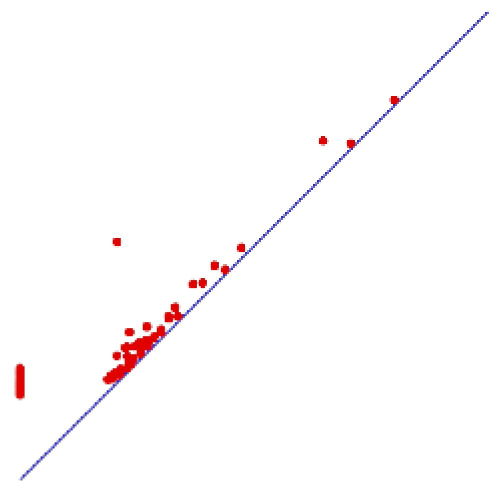

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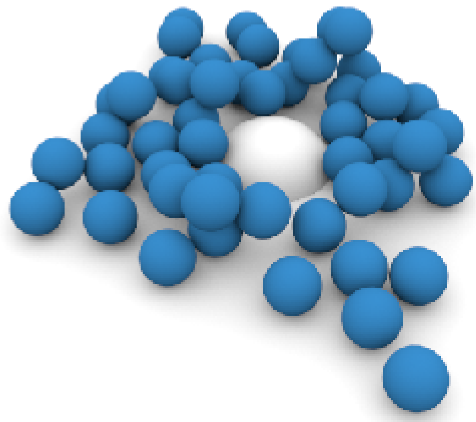

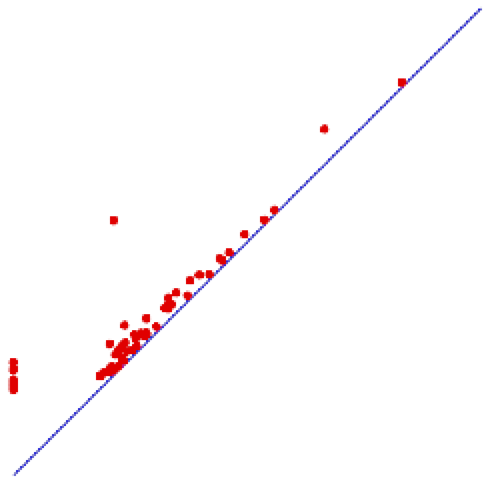

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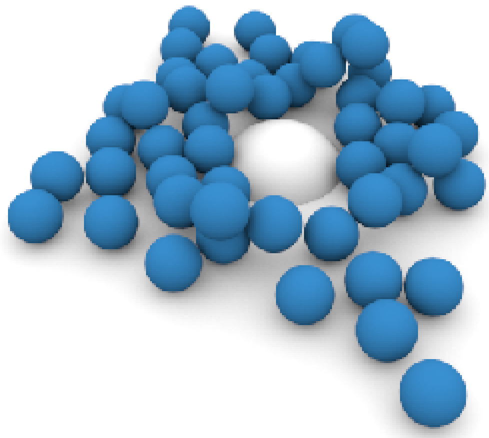

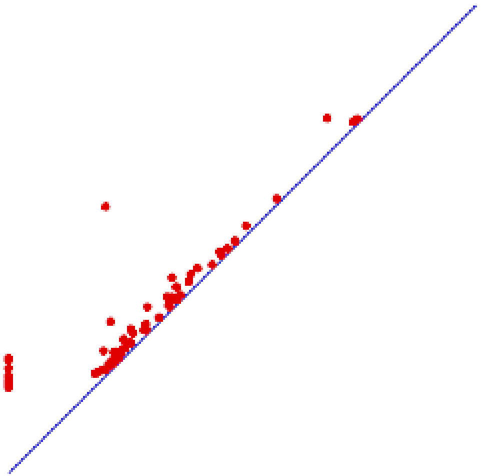

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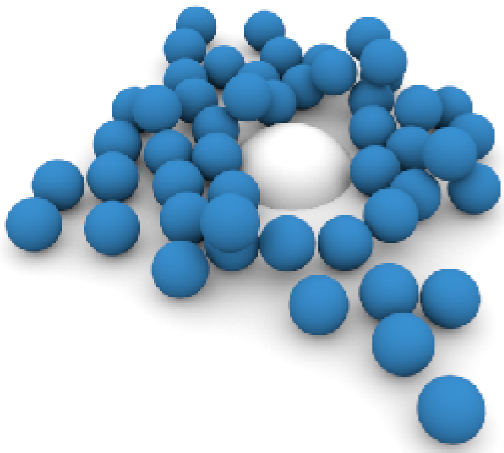

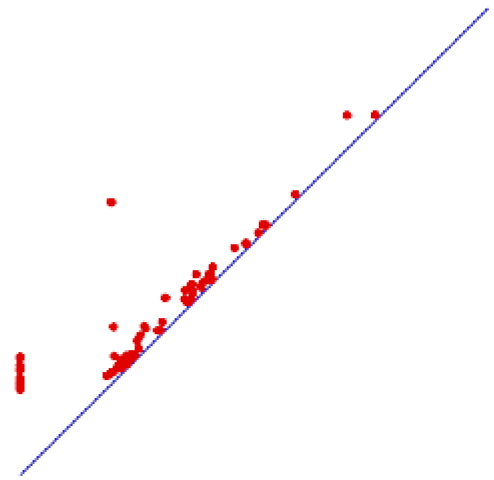

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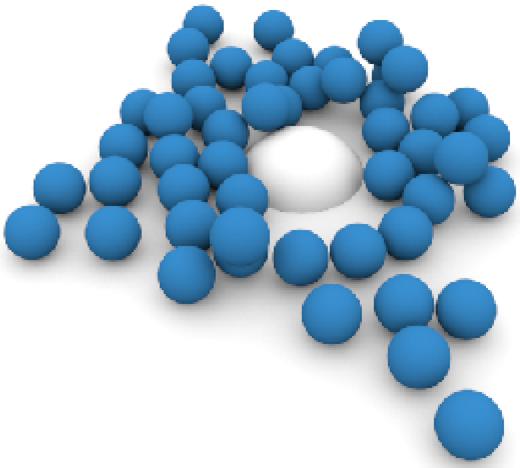

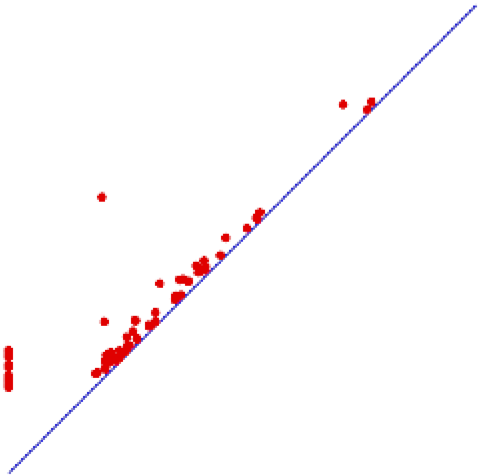

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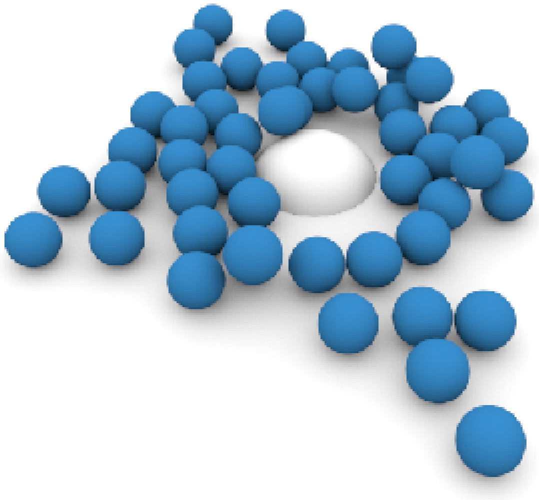

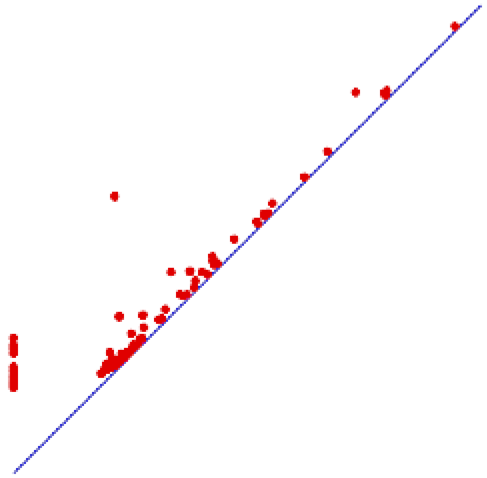

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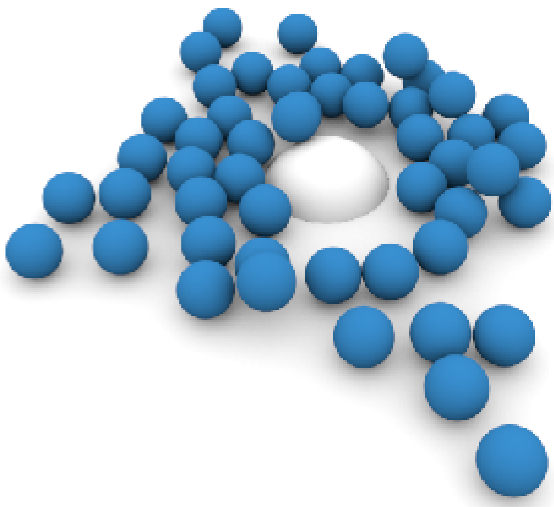

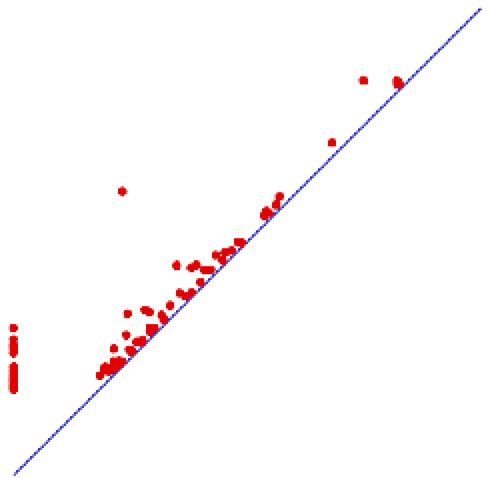

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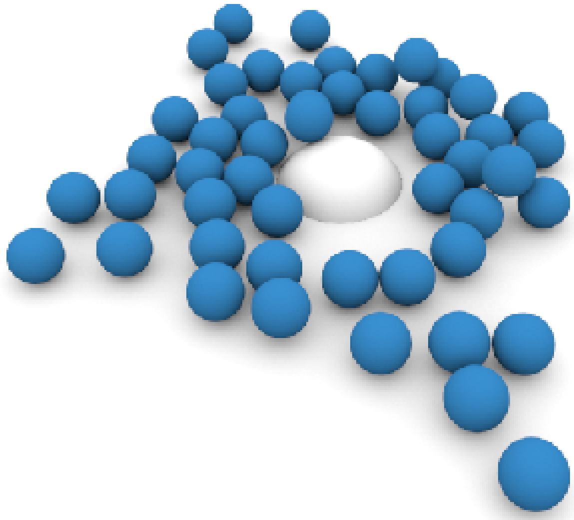

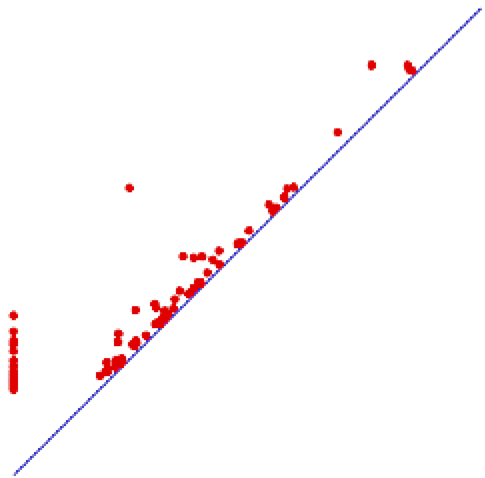

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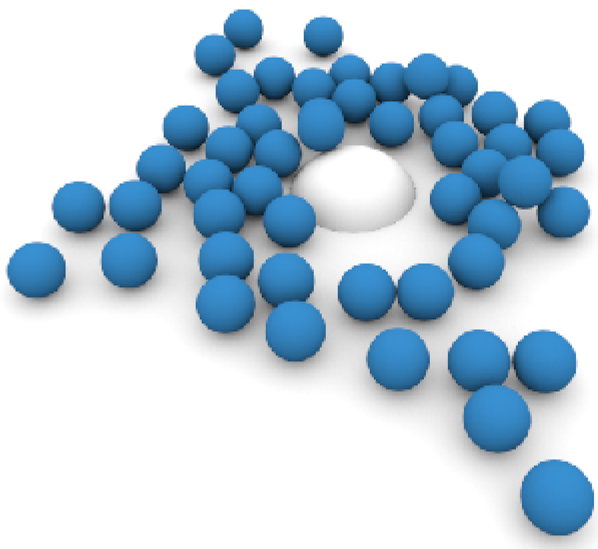

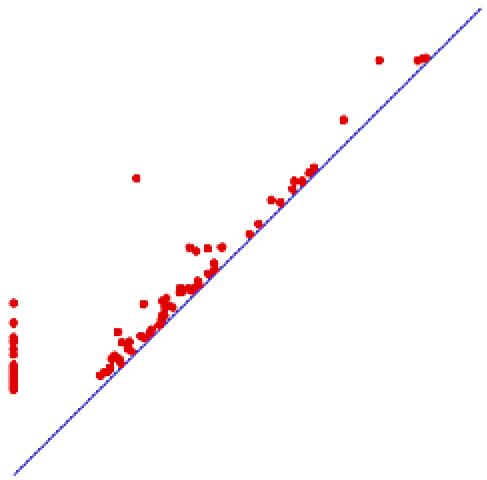

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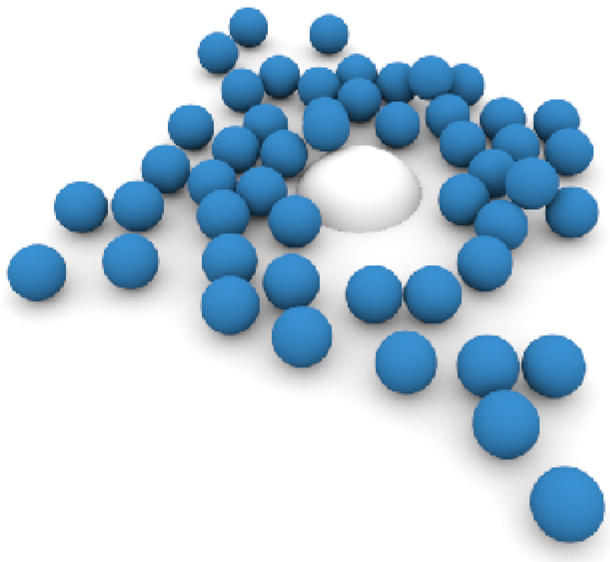

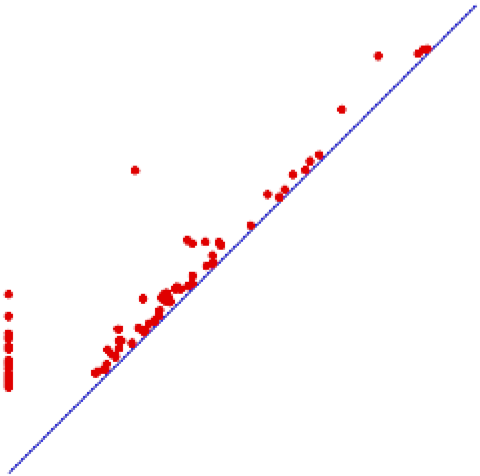

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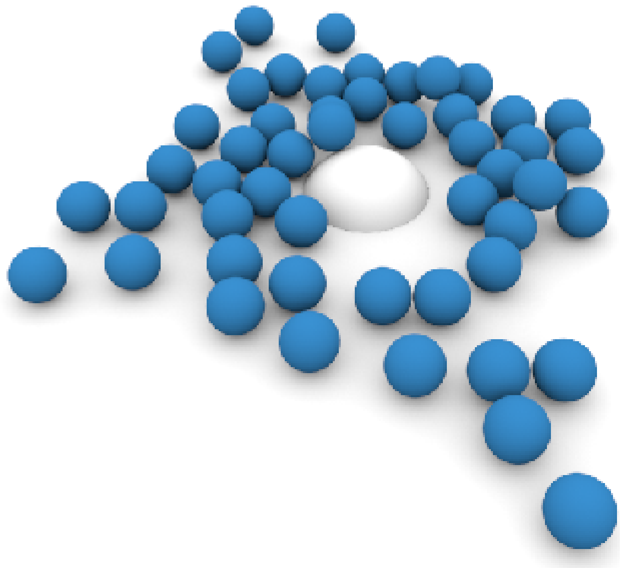

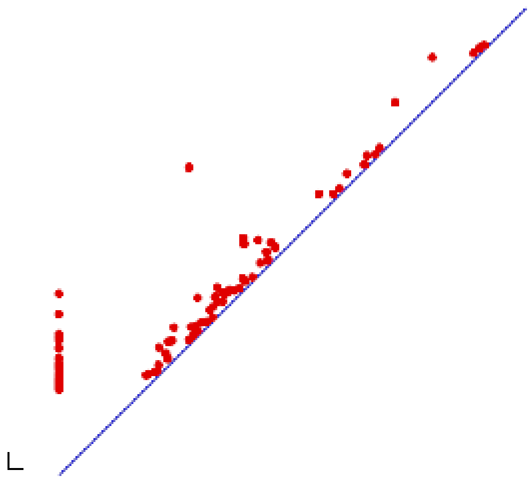

STABILITY

Bottleneck distance between two diagrams is length of longest edge in minimizing matching: $W_\infty(\mathrm{Dgm}(f), \mathrm{Dgm}(g))$

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Thm. $W_\infty(\mathrm{Dgm}(f), \mathrm{Dgm}(g)) \leq \|f-g\|_\infty$.

[Cohen-Steiner, E, Harer 2007]

I BioGeometry

II Wrap

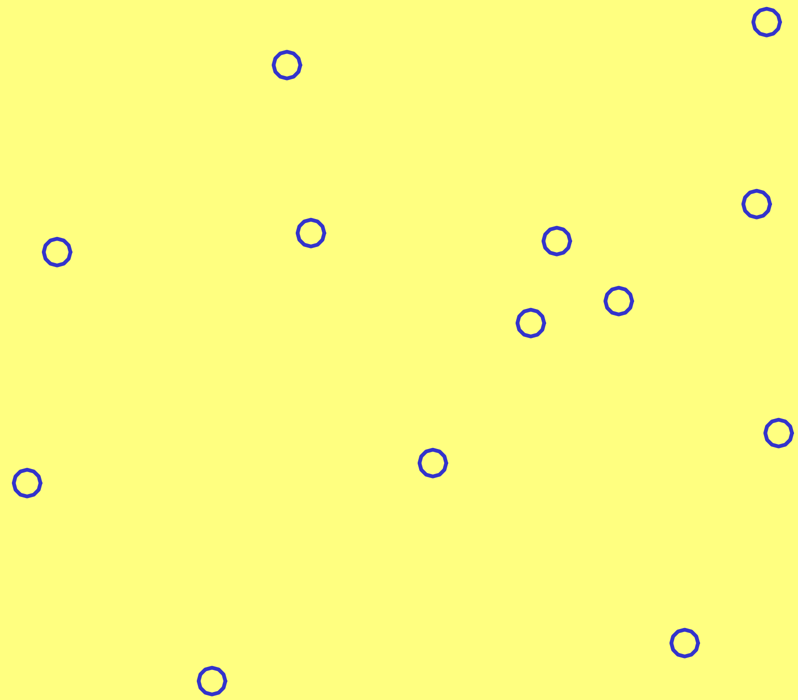
III Persistence

IV Expectation

Poisson Point Process

(with density $\rho > 0$ in $\mathbb{R}^n$)

1. #pts in disjoint sets are independent
2. $\mathbb{E}[\#\text{pts in } B] = \rho \|B\|$



Poisson Point Process

(with density $\rho > 0$ in $\mathbb{R}^n$)

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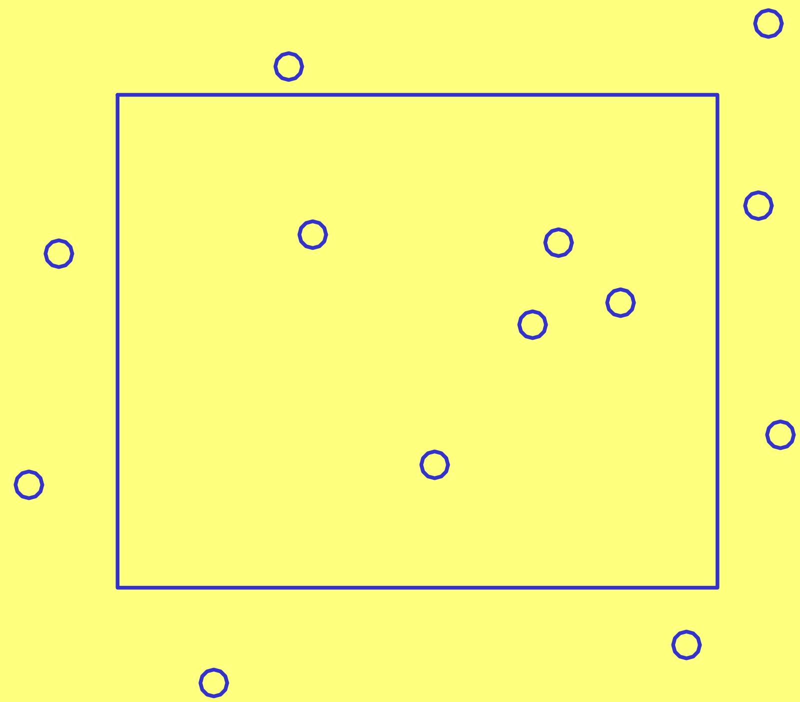

$$\mathbb{P}[\#\text{pts in } B = k] = \frac{(\rho \|B\|)^k}{k!} e^{-\rho \|B\|}.$$

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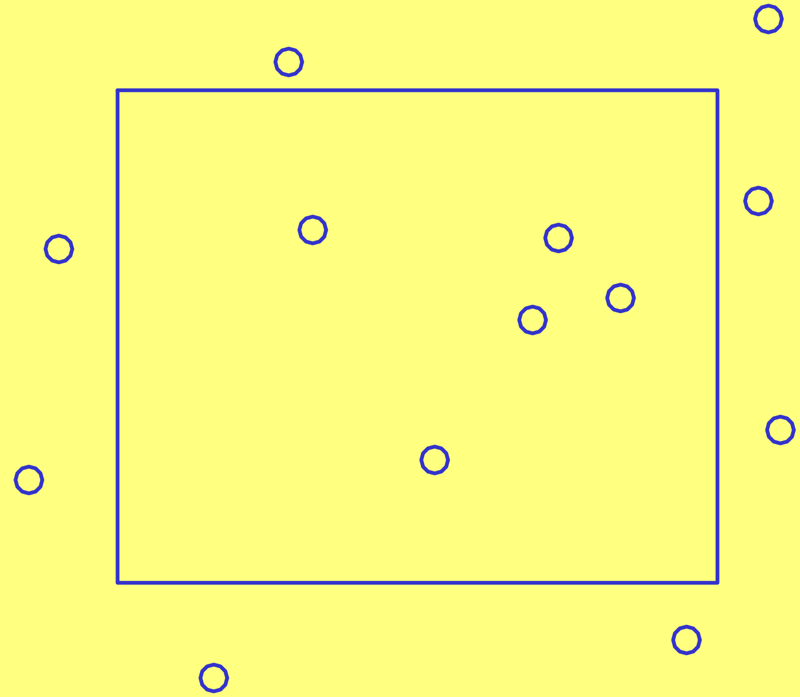

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Points are in general position with prob. 1.

Expectations in $\mathbb{R}^n$

X chosen from PPP with density $\rho > 0$ in $\mathbb{R}^n$.

$\Omega \subseteq \mathbb{R}^n$; $\ell = \dim L$, $k = \dim U$.

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$$\mathbb{E}\left[\#\mathrm{int}_{\ell,k} \text{ in } \Omega \text{ with } r_D \le r\right] = \frac{\gamma(k, \varrho \nu_n r^n)}{\Gamma(k)} \cdot C^n_{\ell,k} \cdot \varrho \|\Omega\|.$$

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[E., Nikitenko, Reitzner 2016]

Critical Simplices and Intervals

$C^2_{\ell,k}$	$k=0$	1	2
$\ell=0$	1		
1		2	1
2			1

$C^3_{\ell,k}$	$k=0$	1	2	3
$\ell=0$	1			
1		4	2.55	1.21
2			4.85	3.70
3				1.85

$C^4_{\ell,k}$	$k=0$	1	2	3	4
$\ell=0$	1				
1		8	5.66	3.55	1.66
2			17.66	18.96	11.14
3				15.40	14.22
4					4.74

Delaunay Simplices

$$\mathbb{E}[\#\, j\text{-simpl. in } \mathrm{Del}] = D_j^n \cdot \varrho \|\Omega\|.$$

$$D_j^n = \sum_{k=j}^{n} \sum_{\ell=0}^{j} \binom{k-\ell}{k-j} C_{\ell,k}^n$$

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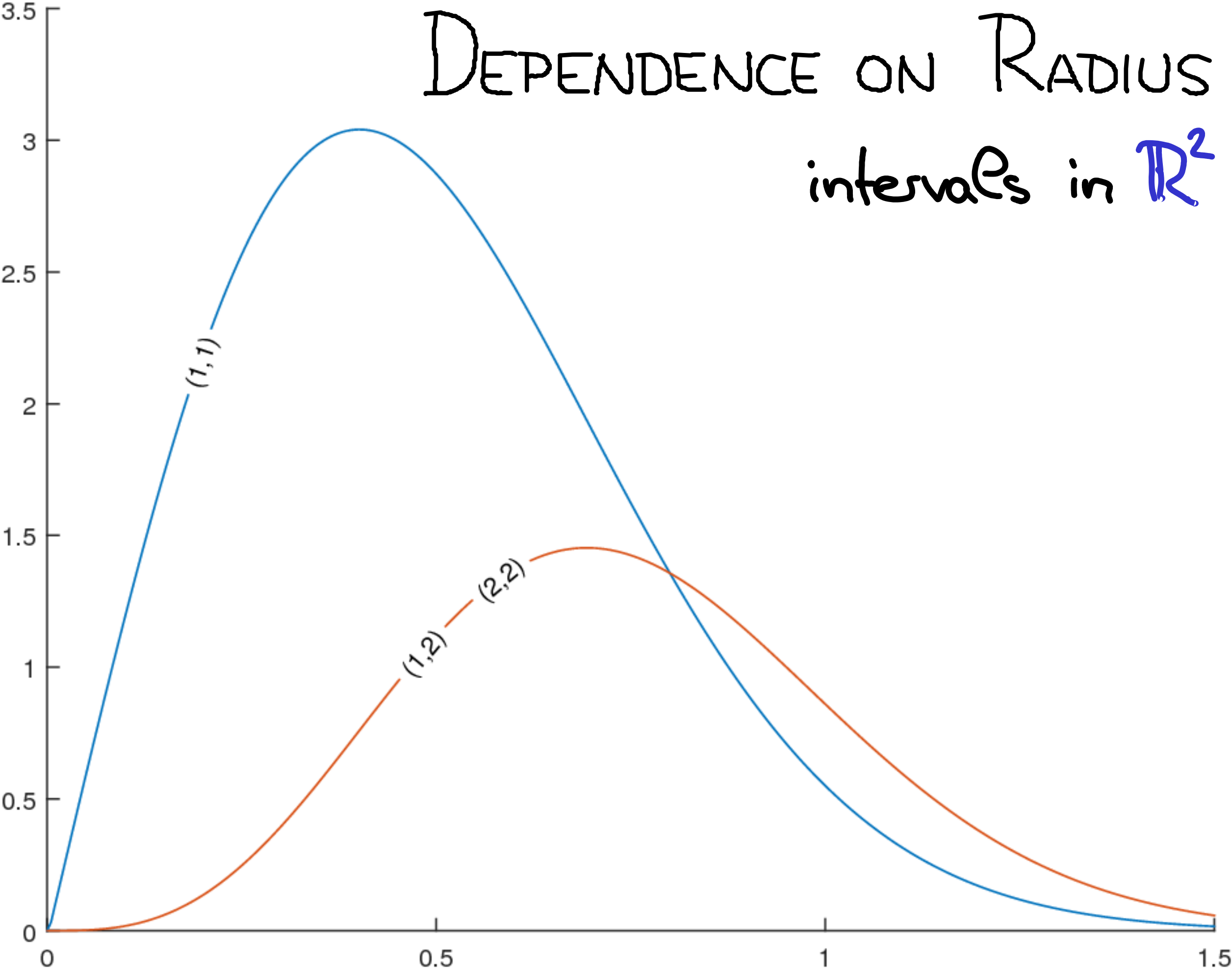
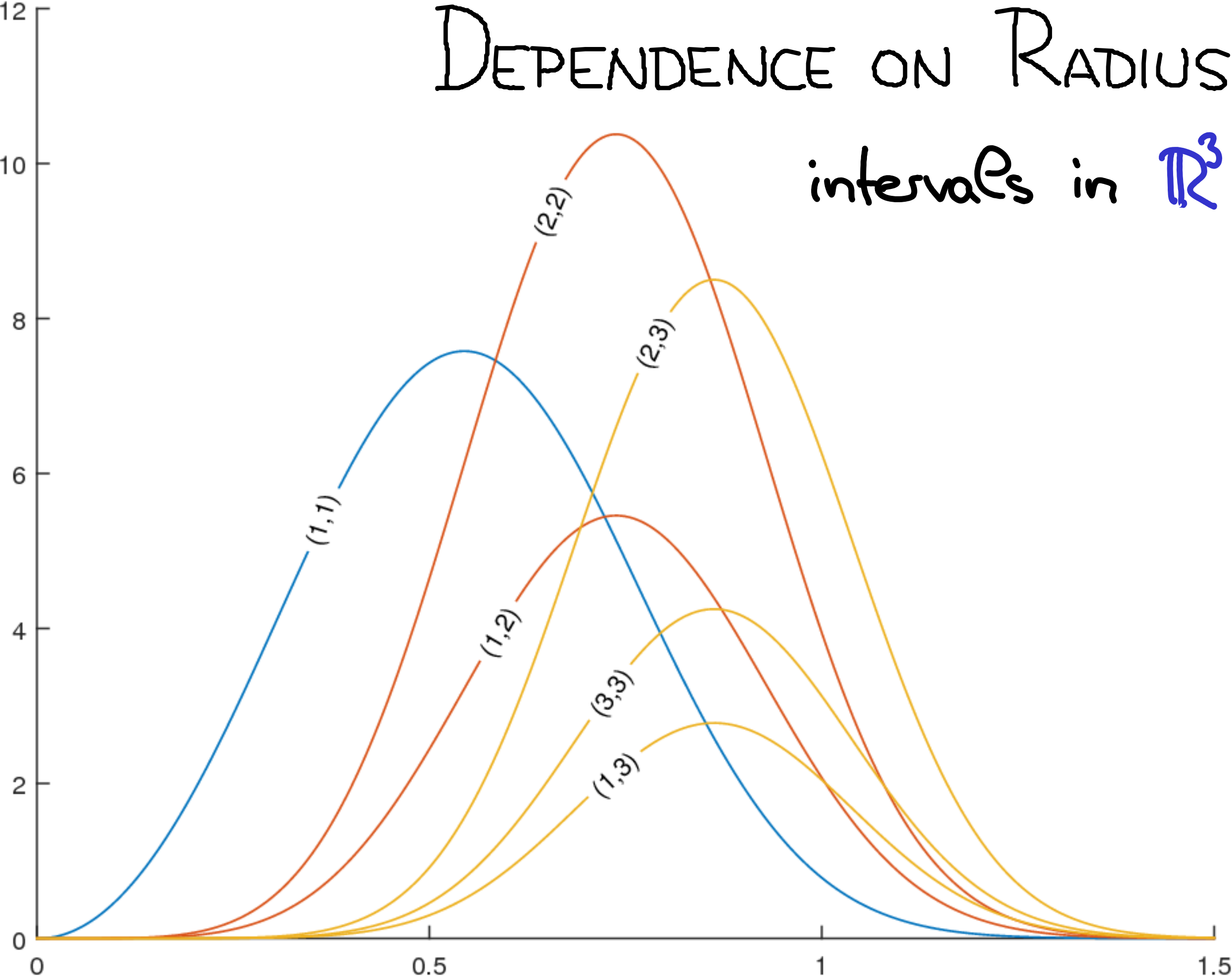
D_j^n	$j=0$	1	2	3	4
$n=2$	1	3	2		
3	1	7.76	13.53	6.76	
4	1	18.88	65.55	79.44	31.77

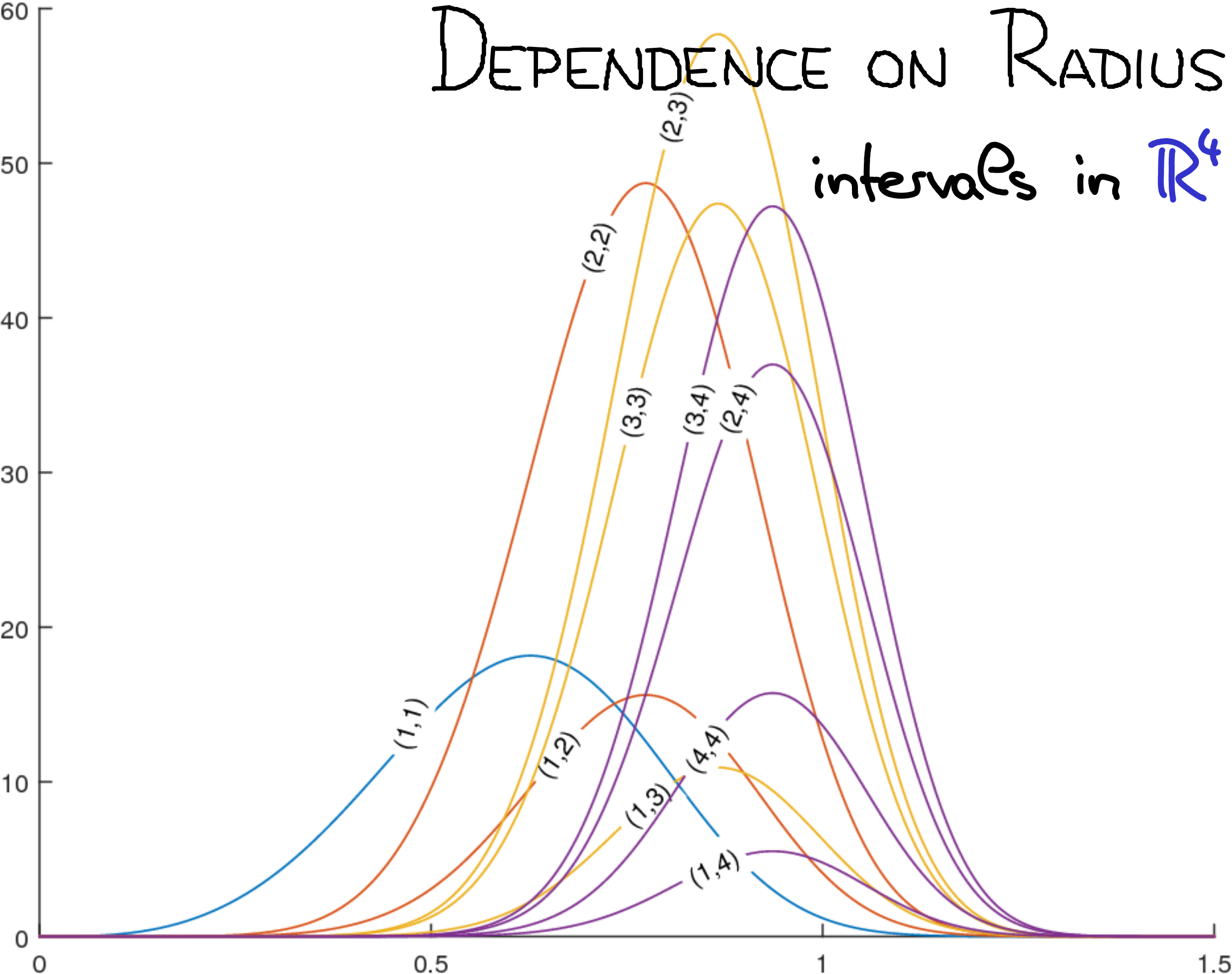
blue = [Miles 1970/71]

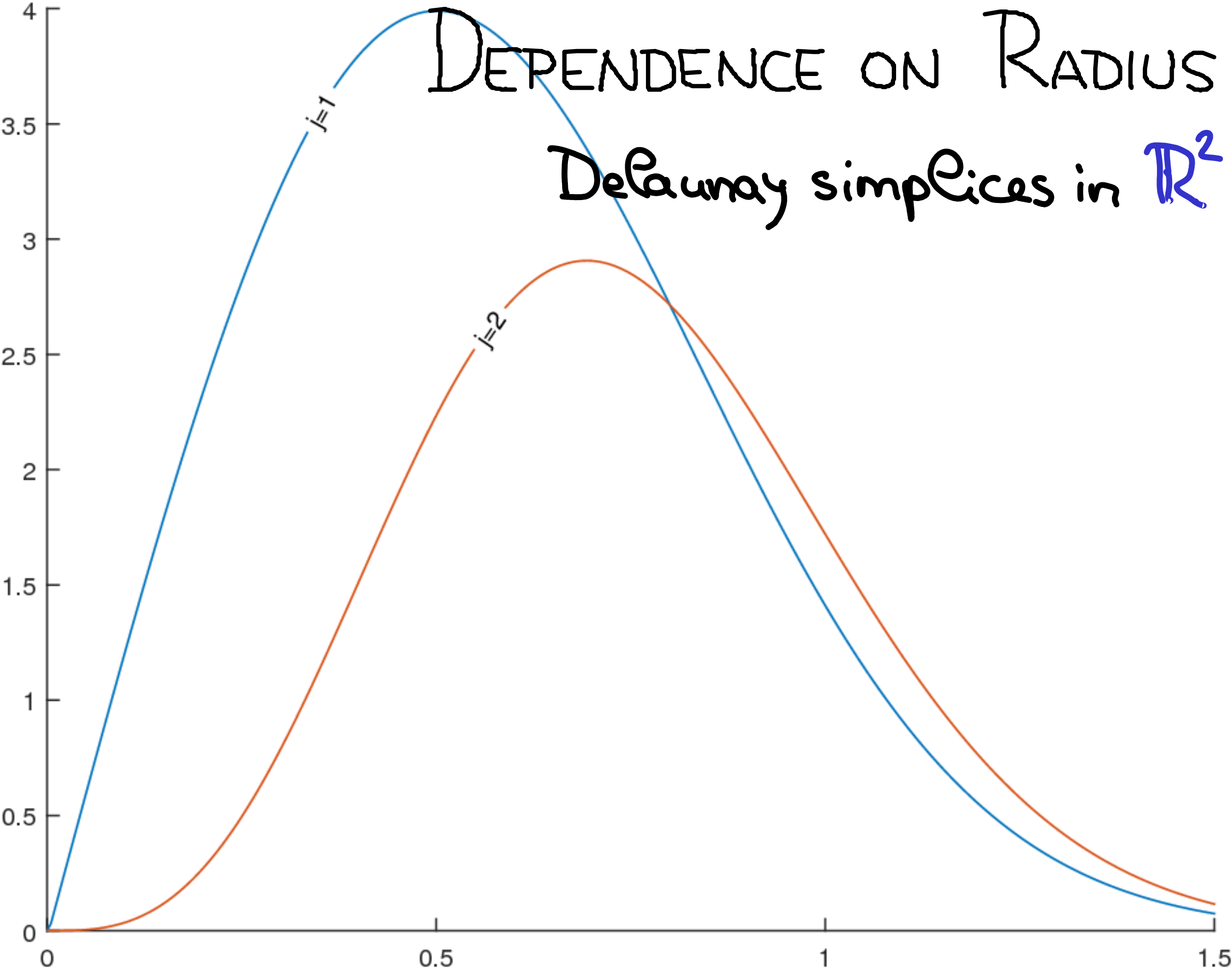
red = [E, Nikitenko, Reitzner 2016]


Dependence on Radius
intervals in $\mathbb{R}^2$
(1,1)
(1,2)
(2,2)
0
0.5
1
1.5
2
2.5
3
3.5
0
0.5
1
1.5



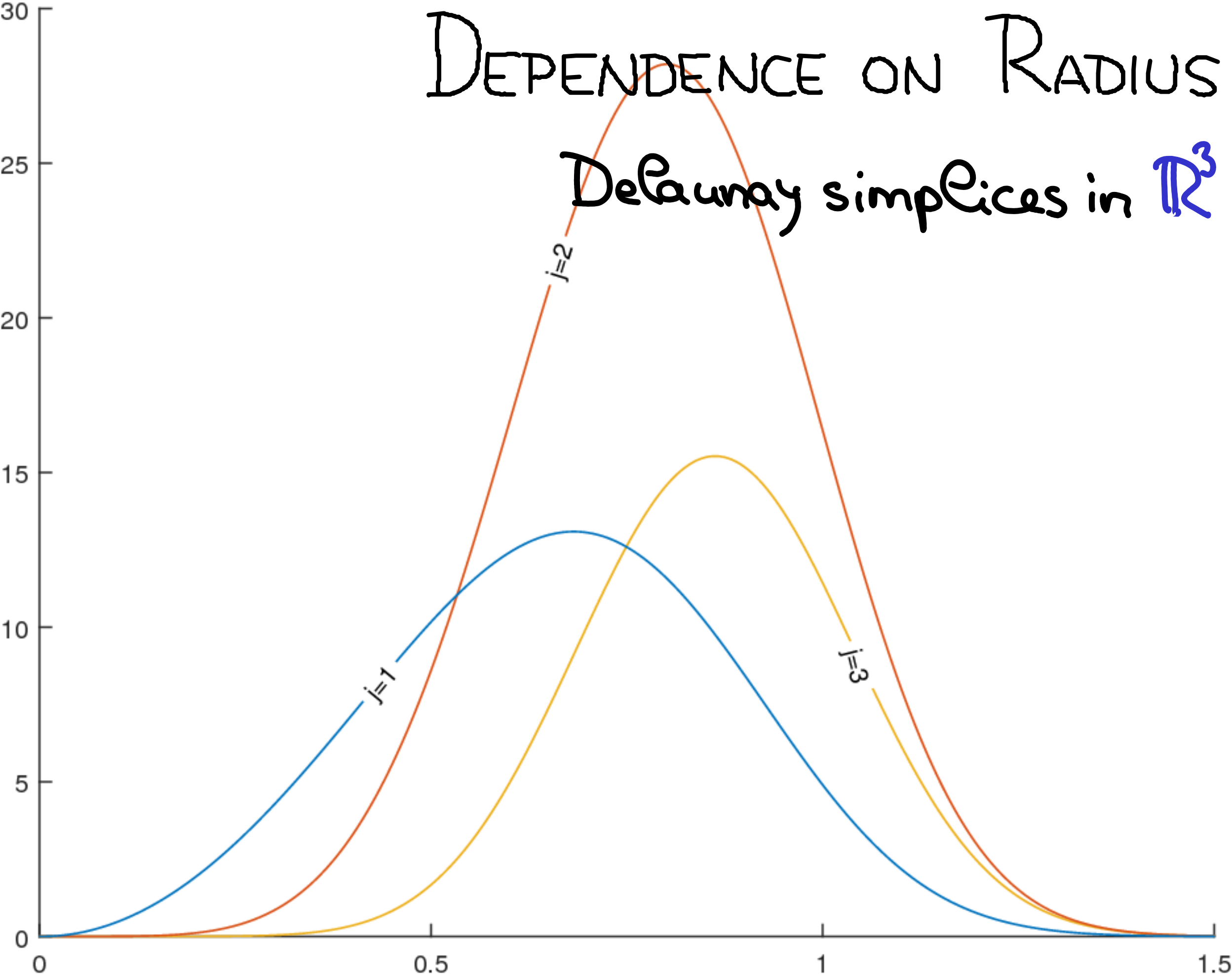
Dependence on Radius
intervals in $\mathbb{R}^3$
(1,1)
(2,2)
(1,2)
(2,3)
(3,3)
(1,3)
0
2
4
6
8
10
12
0
0.5
1
1.5


Dependence on Radius
intervals in $\mathbb{R}^4$
(1,1)
(1,2)
(1,3)
(1,4)
(2,2)
(2,3)
(2,4)
(3,3)
(3,4)
(4,4)
0
10
20
30
40
50
60
0
0.5
1
1.5


Dependence on Radius
Delaunay simplices in $\mathbb{R}^2$
j=1
j=2
0
0.5
1
1.5
2
2.5
3
3.5
4
0
0.5
1
1.5

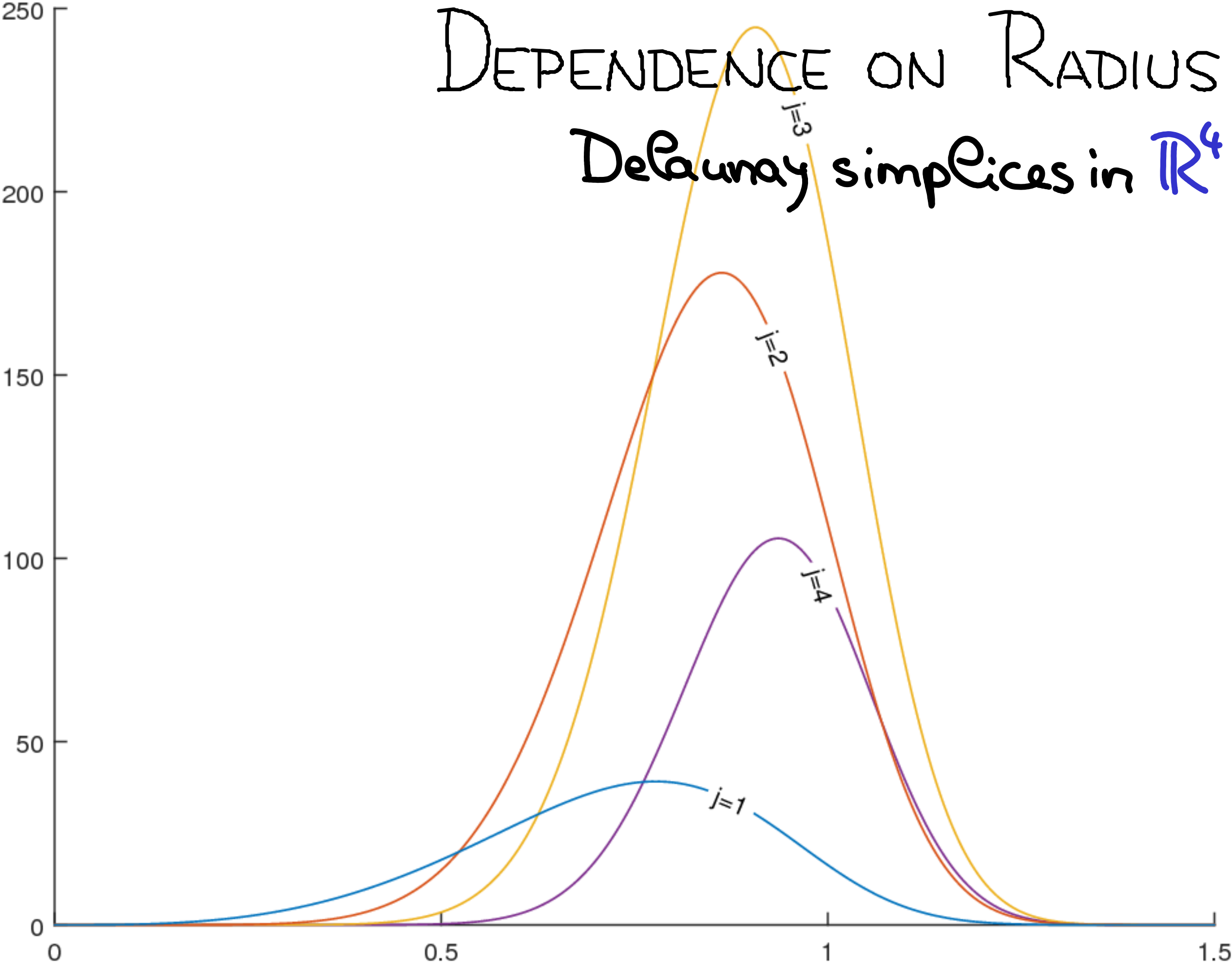
Dependence on Radius

Delaunay simplices in $\mathbb{R}^3$

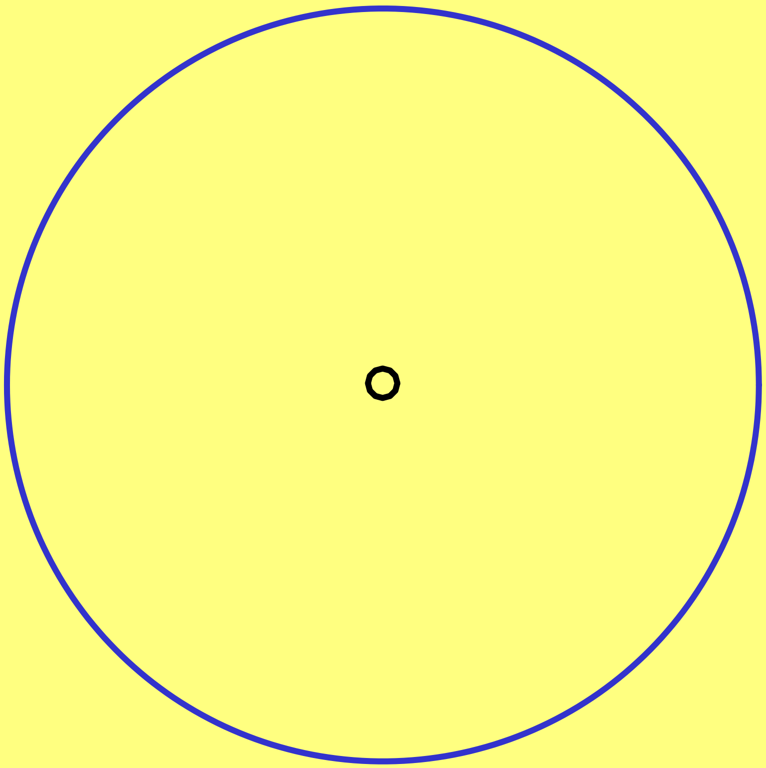


Dependence on Radius

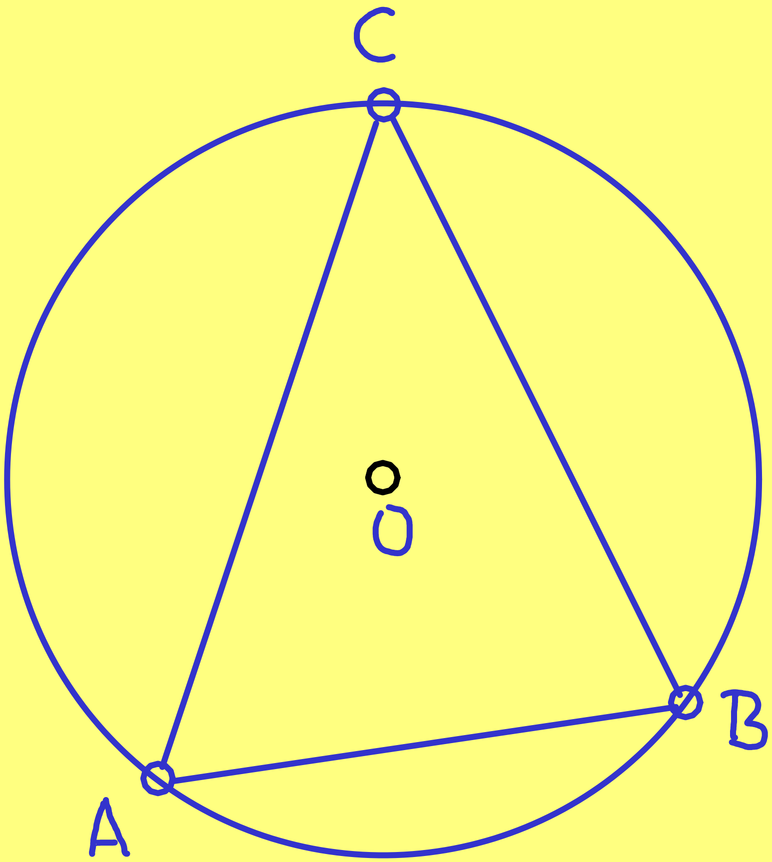
Delaunay simplices in $\mathbb{R}^4$



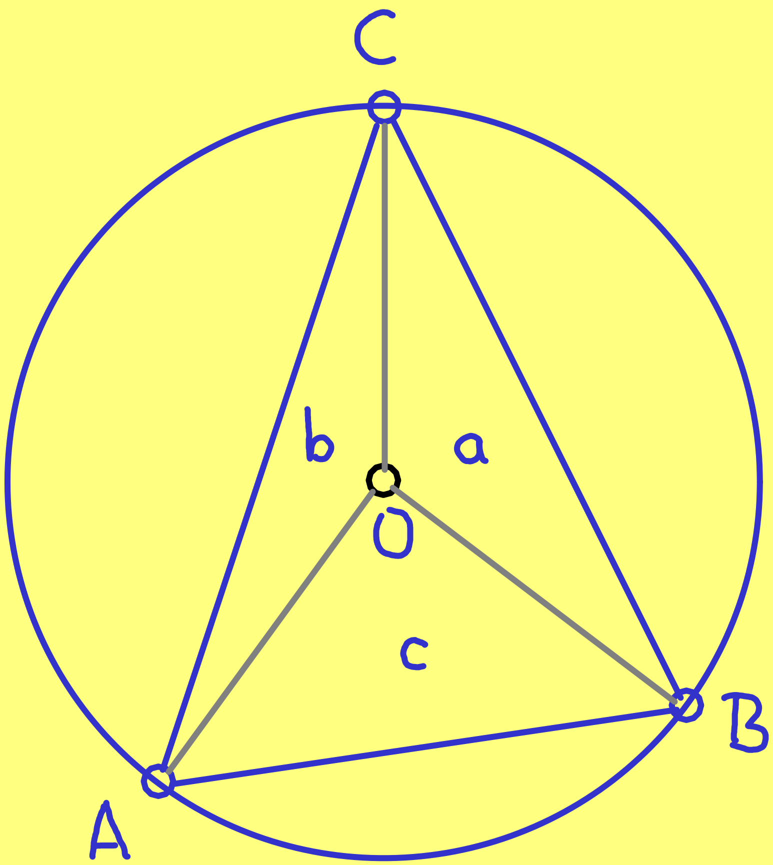
Three Points on Circle



Three Points on Circle

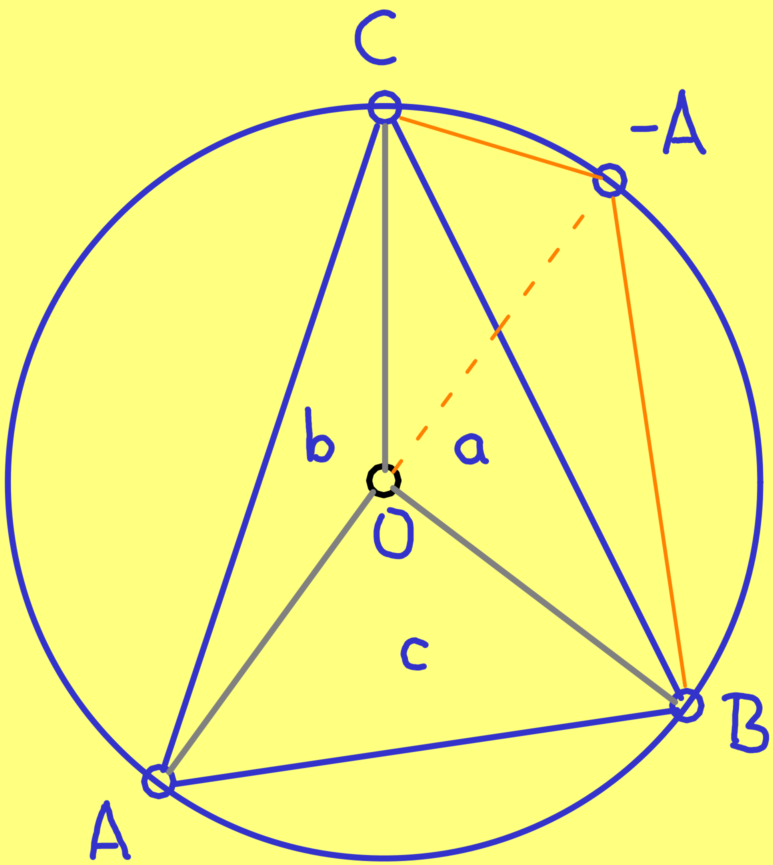


Three Points on Circle



area(ABC) = a+b+c

Three Points on Circle

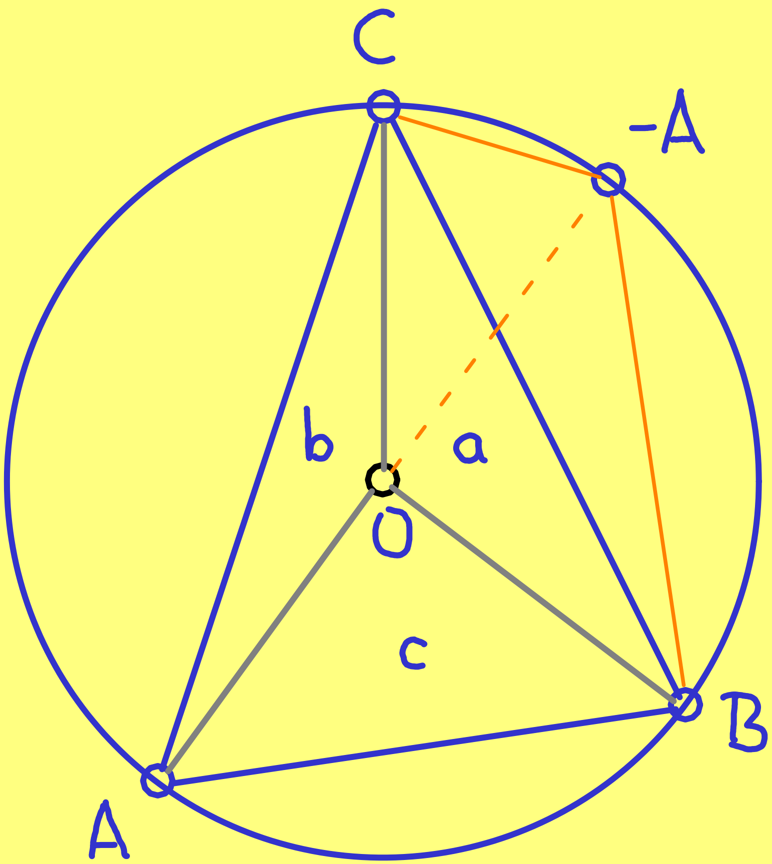


$$\text{area}(ABC) = a + b + c$$

$$-ABC = -a + b + c$$

Three Points on Circle

[Wendel 1963]



area(A B C) = a + b + c

-A B C = -a + b + c

A -B C = a - b + c

A B -C = a + b - c

-A -B C = -a - b + c

-A B -C = -a + b - c

A -B -C = a - b - c

-A -B -C = -a - b - c

THANK YOU