

# From polygons and museums to molecules and massive data

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Geometry in the Computer

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#### Overview

#### Museums and Triangles

#### Molecules

#### Massive

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# Antiquity





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# Continuous vs Discrete





# Outline

#### Museums and Triangles

Molecules

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#### Museum Guards



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#### Art gallery Theorems: a classic

- Minimizing the number of point-guards to cover a simple polygon is NP-hard.
- ▶ In general,  $\lfloor n/3 \rfloor$  guards cover a *n*-gon.
- The main algorithmic step is triangulation. It is in O(n): deterministic [Chazelle], or simpler randomized algorithm.



► Applications: visibility, telecom networks, extension to 3D.

The best triangulation ...



#### Boris Delaunay [1934]

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#### ... equivalent to a distance partition





# Graphics



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# Computational Geometry Algorithms Library



- Efficient algorithms
- Exact computation
- ► C++ / STL library
- Open project, mostly European

# CGAL triangulation / mesh



## CGAL convex hull / arrangement





# Outline

#### Museums and Triangles

#### Molecules

Massive

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#### Dogma



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# Docking





 $\alpha \text{-shapes:}$  success story and major tool in bioinformatics









#### 3D structure



# CGAL



# $\text{Different } \alpha$



#### [Edelsbrunner]

# Outline

Museums and Triangles

Molecules

#### Massive

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#### 3D



 $http://www.youtube.com/watch?v{=}OqVNQmX\_J28$ 

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# Databases



# Approximate Voronoi diagram



https://github.com/akonskarm/AVD

#### Data structures: towards data mining



 $\epsilon$ -nearest neighbor in msec among 1M points in > 100 dimensions.

#### Curse of dimensionality

Tree based methods, e.g. AVD: For fixed *d*, space =  $O(n/\epsilon^d)$ ,  $\epsilon$ -nearest neighbor in  $O(\log(n/\epsilon))$ . [Mount, Har-Peled, et al.]

Locality sensitive hashing: polynomial-time in d, exponential in  $\epsilon$ . [Indyk, Motwani, et al.]

#### High dimensions: towards structure

# Bioinformatics, the Internet, GIS, Image processing: they all easily provide data in e.g. 100, or 1000 dimensions.





#### Current goal: Exploit structure [Guibas]

#### And then?



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