APPLIED aspects of COMPUTATIONAL GEOMETRY

Spherical Arrangements, Union Boundary, Sparsity

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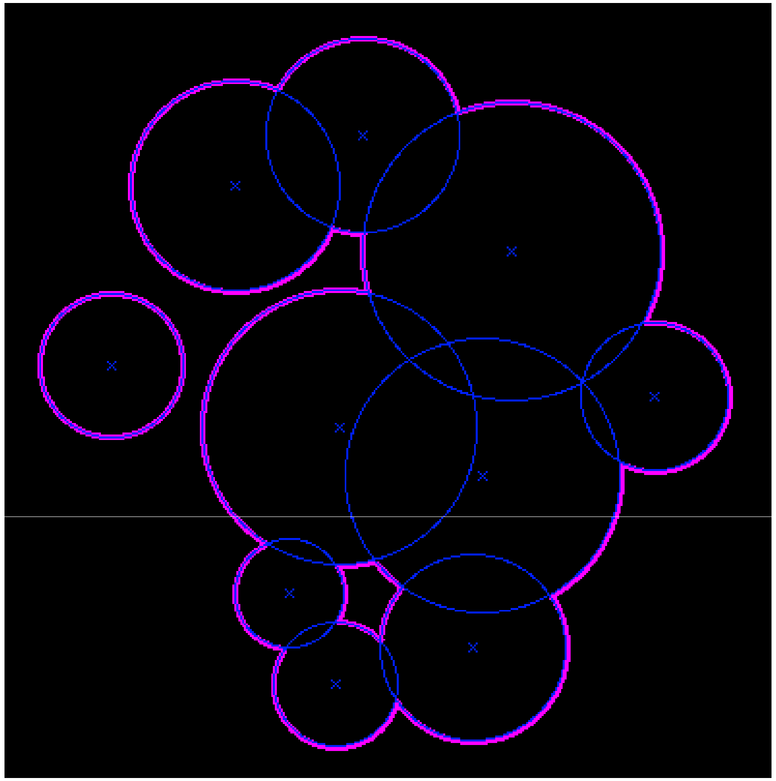
Overview

- spherical arrangements
- another substructure: union boundary
- favorable (sparse) arrgs: atom spheres
- arrgs with low stabbing number

Arrgs of spheres

- arrgs of circles, complexity
- arrgs of spheres, complexity
- another substructure in arrangements of surfaces bounding regions:
  the union boundary

Arrgs of circles, the union boundary



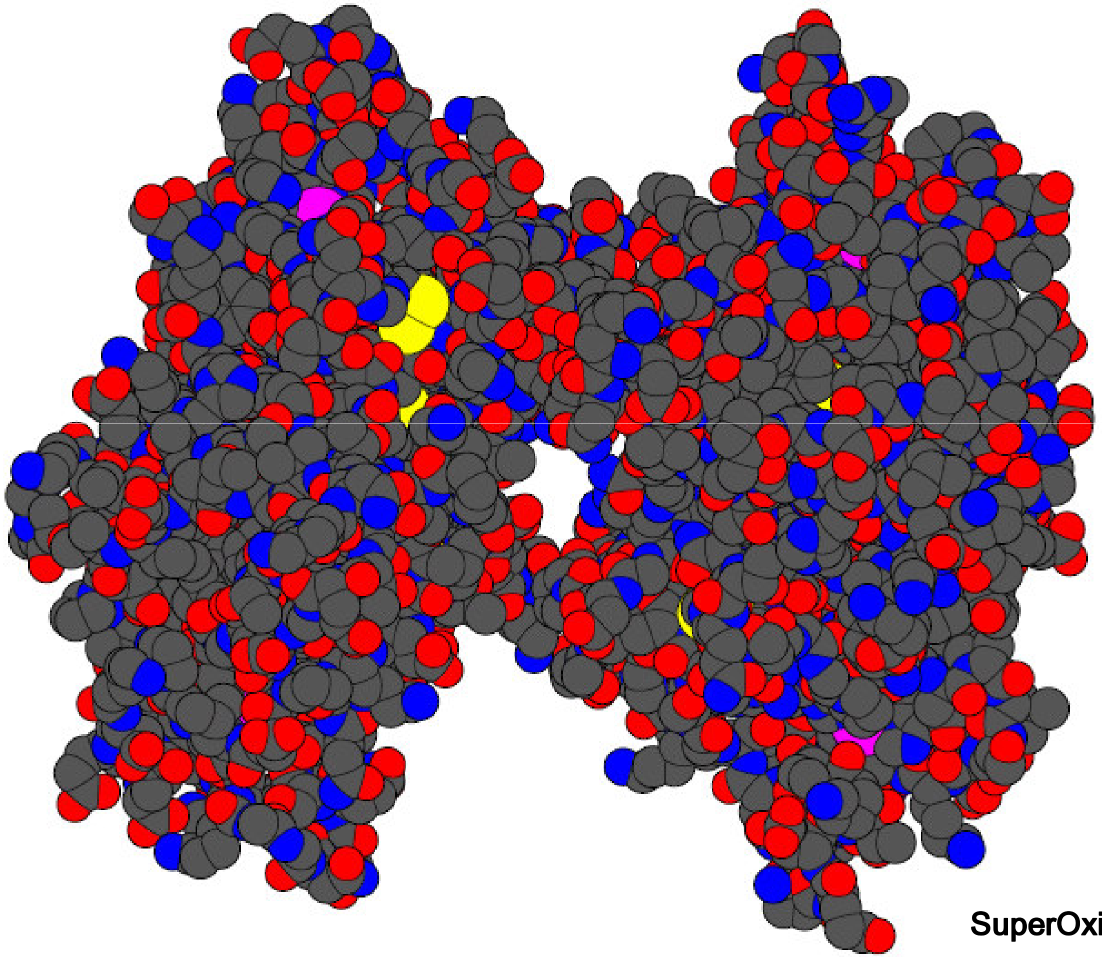
how complex?

- the number of vertices on the boundary of the union of n ≥ 3 disks in the plane is at most 6n-12 and this bound is tight [pf]
- the complexity of the union boundary of n d-balls in R^d is $O(n^{\lceil d/2 \rceil})$, in particular in R^3 it is $\theta(n^2)$

Proof (union boundary complexity, circels)

- the lifting transform onto the unit paraboloid $z=x^2+y^2$
- each transformed circle is contained in a plane
- the union boundary: on the paraboloid, above the upper envelope of the planes
- the complexity of the upper envelope of n planes: $E=V+F-2=V+n-2 \leq 2/3E+n-2$
- each edge of the upper envelope contributes at most two vertices to the union boundary
- the bound is tight

A favorable arrg of spheres: arrg of atoms in a molecule



SuperOxide Dismutase, 4932 atoms

The union boundary of a molecule

- complexity
- construction
- drawing

- vertical decomposition of the arrangement:
  - inside spheres
  - outside spheres

Complexity

Theorem 2.1. *Let $M = \{B_1, \ldots, B_n\}$ be a collection of n balls in 3-space with radii $r_1, \ldots, r_n$ and centers at $c_1, \ldots, c_n$. Let $r_{\min} = \min_i r_i$ and let $r_{\max} = \max_i r_i$. Also let $S = \{S_1, \ldots, S_n\}$ be the collection of spheres such that S_i is the boundary surface of B_i. If there are positive constants k, ρ such that $r_{\max}/r_{\min} < k$ and for each B_i the ball with radius $\rho \cdot r_i$ and concentric with B_i does not contain the center of any other ball in M (besides c_i), then:*

(i) *for each $B_i \in M$, the maximum number of balls in M that intersect it is bounded by a constant,*

(ii) *the maximum combinatorial complexity of the boundary of the union of the balls in M is $O(n)$.*

$$\frac{(r_i + 2r_{\max})^3}{(\frac{\rho}{2} \cdot r_{\min})^3} \le \frac{(3r_{\max})^3}{(\frac{\rho}{2} \cdot r_{\min})^3} \le 216 \cdot (\frac{k}{\rho})^3$$

molecule	k	ρ	max	aver.
caffeine	2.17	0.71	10	4.5
acetyl	3.11	0.67	16	5.4
crambin	1.64	0.78	10	5.5
felix	1.64	0.81	9	4.9
SOD	1.95	0.76	16	5.5

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Robust construction with floating point

- controlled perturbation: certified, degeneracy-free geometric computing with fixed precision arithmetic
- applied to arrgs of circles, spheres, segments, to Delaunay triangulations, and more

Other sparse arrgs

- arrgs with low vertical stabbing number
  n curves/surfaces, vertical stabbing k
  - in the plane

  $O(nk)$
  - in 3-space

  $O(n^2k)$ for a proof, see [dBHOvK]
- arrgs of k polytopes with a total of n facets

  $O(nk^2)$
- all the bounds above are tight
- motivation: for low-vertical-stabbing---visibility over a terrain, for arrgs of polytopes---assembly partitioning (later)

References

- [H-Overmars '98]
  Spheres, molecules, and hidden surface removal, CGTA
- [H-Shelton '98]
  A perturbation scheme for spherical arrangements with application to molecular modeling, CGTA
- [H-Leiserowitz '04]
  Controlled perturbation for arrangements of circles, IJCGA
- [de Berg-H-Overmars-van Kreveld '97]
  Sparse arrangements and the number of views of polyhedral scenes, IJCGA

- CGTA = Computational Geometry, Theory & Applications
- IJCGA = Intn'l Journal of Computational Geometry and Applications

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