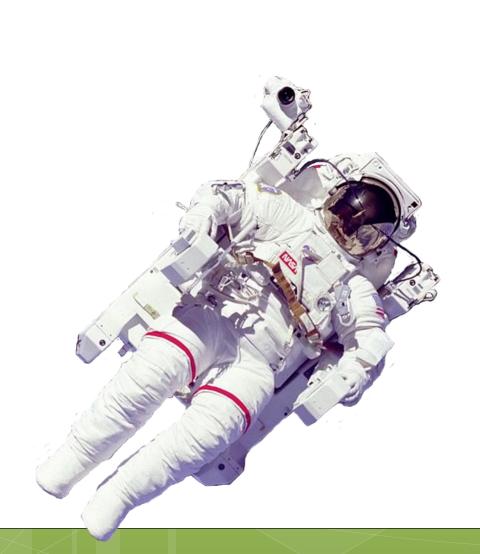
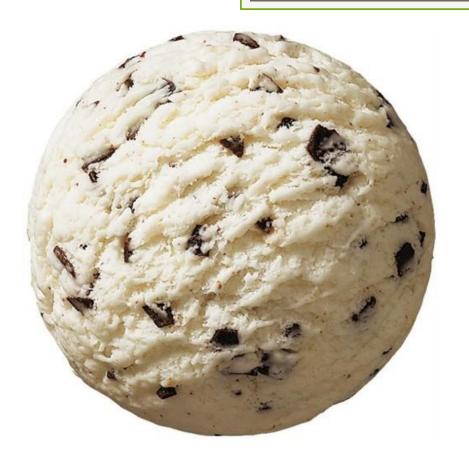


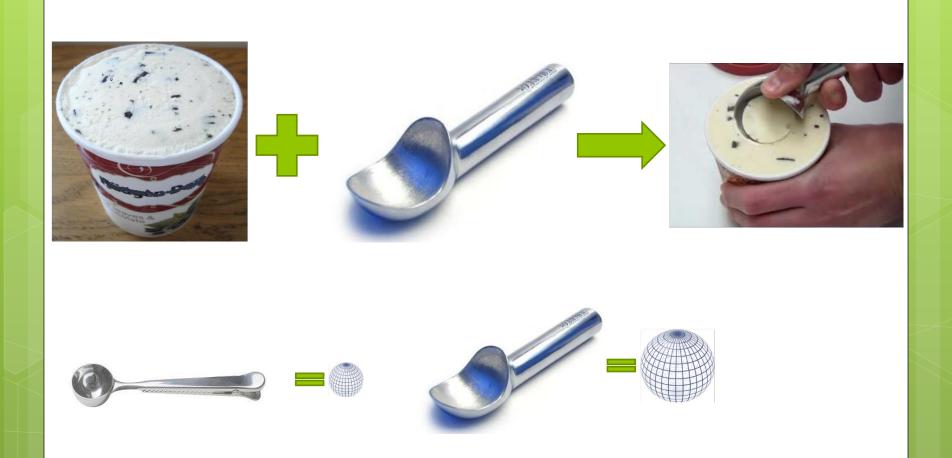
Weighted a-shapes

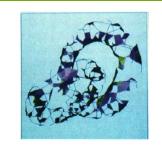
Νίκος Μπεγέτης ΠΙΒ0111

- Multi-scale Geometric Modeling of Ambiguous Shapes with Tolerance Balls and Compoundly Weighted a-shapes
 - Frédéric Cazals Tom Dreyfus
- Weighted Alpha Shapes
 - Herbert Edelsbrunner



















Introduction

- Protein Structure

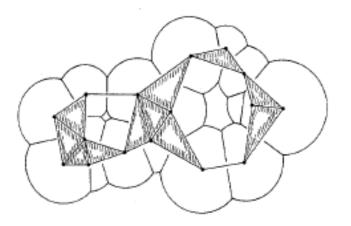
 Molecular function
- Pockets (θύλακες)
 - Regions in the complement, limited from the outside
 - Efficiently created with the a-shapes algorithm
- Cavities (Κοιλότητες), Gorges (Χαράδρες)

Spherical Ball Models

- Space filling model (Waals radii)
 - Distance and growth
 - Spherical ball → atom
 - Union of spherical balls → facets
 - Outside
 - Voids
- Solvent Accessible Models
 - Weighted balls: different size, same center
 - Ball expansion
 void contraction

Alpha Complexes

- a-complex: 2 disks in 2-dim or 2 spheres in 3-dim abutting
- 2 disks centers joined with edges
- 3 disk centers joined with triangles



Regular

Same level of detail in in all parts of space

Weighted

- Different level of detail in different parts of space
- Superset of regular a-shapes:
 - o set w-parameter=0

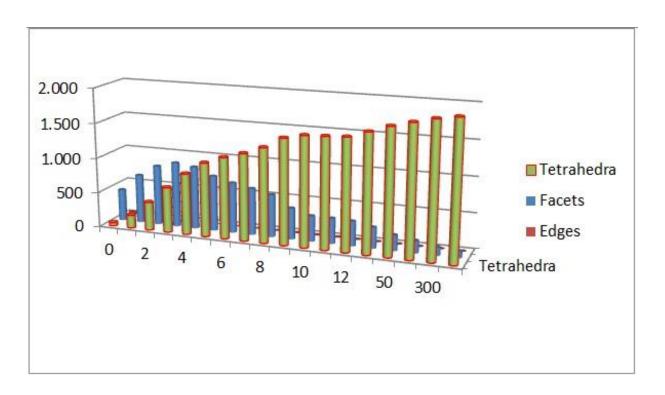
Benefits

- Biology and Chemistry
 - Modeling of molecular structures: model atoms with different van der Waals radii
 - Surface reconstruction: variety of density.
 - If regular a-shapes with big a-parameter → hidden details in dense regions.
 - Alternatively, with small parameter holes and sparse regions.
 - Solution: large weight in sparse regions and small in dense regions
 - Enforce edges or faces and begin with these given as input, not only a point set input

a-shapes in CGAL

- Delaunay & Regular Triangulation
- O CGAL::Alpha_shape_3<Dt,ExactAlphaComparisonTag>
 - CGAL library for a-shapes
 - CGAL::object
 - Type used to sort points in the complex while a parameter is growing
 - Functions:
 - Finding links
 - given a-parameter no. of types found: points, edges, faces, polyhedra
 - Dt = triangulation used for this example
 - ExactAlphaComparisonTag = true/false is facet belongs in acomplex of points respectively

Code Implementation in given protein coordinates



• Best a-parameter: 11.1103

Misc - Links

Useful links and papers

- Multi-scale Geometric Modeling of Ambiguous Shapes with Tolerance Balls and Compoundly Weighted a-shapes: Frédéric Cazals – Tom Dreyfus
- Weighted Alpha Shapes: Herbert Edelsbrunner
- http://www.cs.duke.edu/~edels/Papers/1998-J-03-PocketsMacromolecules.pdf : paper introducing a-shapes
- http://www.cs.duke.edu/~edels/: Helbert Edelsbrunner personal site
- http://www.cs.jhu.edu/~misha/Fall05/09.20.05.pdf : Edelsbrunner presentation in a-shapes
- http://www.mpi-inf.mpg.de/~jgiesen/tch/sem06/Celikik.pdf : another very good presentation in a-shapes
- http://cgi.di.uoa.gr/~compgeom/pycgalvisual/cgalvisual/project.pdf : implementation of a-shapes in general from a collegue
- http://cgi.di.uoa.gr/~compgeom/pycgalvisual/cgalvisual.shtml : school site
- http://cgm.cs.mcgill.ca/~godfried/teaching/projects97/belair/alpha.html : example
- http://www.sai.msu.su/sal/E/1/ASVS.html : Helbert Edelsbrunner ALVIS software
- http://www.loria.fr/~pougetma/software/alpha_shape/alpha_shape.html : opensource software
- http://sts-fw.bioengr.uic.edu/castp/examples.php: synchronous software company affiliated with molecular biology
- http://www.cs.duke.edu/~edels/Publications/Alpha/: other useful papers

Thank you for your attention!