Informatica Biomedica
lezione18

Alberto Paoluzzi Mauro Ceccanti
www.dia.uniroma3.it/ paoluzzi/web/did/biomed/

Informatica e Automazione, "Roma Tre" — Medicina Clinica, "La Sapienza"

May 17, 2010

Fonte essenziale: Chapter 9 of book: J. Gu and P.E. Bourne, *Structural Bioinformatics*, Wiley (2009)

Molecular Visualization

α-shapes

Sir John Kendrew with the model of insulin.

The model of insulin was one of the first protein structures to be determined by X-ray crystallography

Prediction of threedimensional structure

The geneticists now believe that the hereditary material determines only the amino acid sequence of a protein, not its 3D structure. That is to say, the polypeptide chain, once synthesized, should be capable of folding itself up without being provided with additional information. If the postulate is true it follows that one should be able to predict the threedimensional structure of a protein from a knowledge of its amino acid sequence alone.
Indeed, in the very long run, it should only be necessary to determine the amino acid sequence of a protein, and its 3D structure could then be predicted; in my view this day will not come soon, [] and it will also be possible to discuss the structures of many important proteins which cannot be crystallized and therefore lie outside the crystallographer's purview.

Myoglobin and the structure of proteins. (1962) Nobel Lecture
– John C. Kendrew

A typical fragment of electron density and a section of atomic model
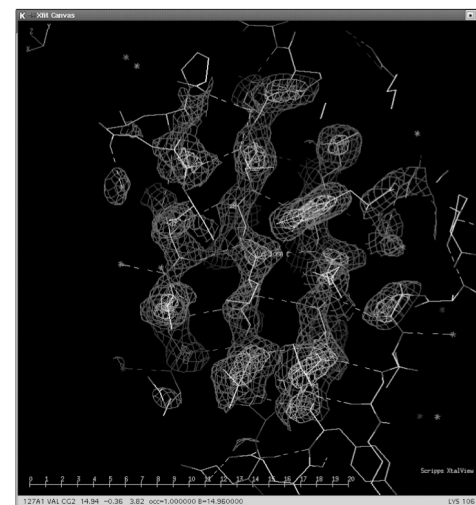

the structure of the CuA domain from cytochrome BC3 (PDB ID code 2CUA), displayed using XFit from XtalView package. Bonds are colored according to the atoms that they join. Putative hydrogen bonds are drawn as dashed white lines.

## Visualization of surface (globular protein 8GCH)
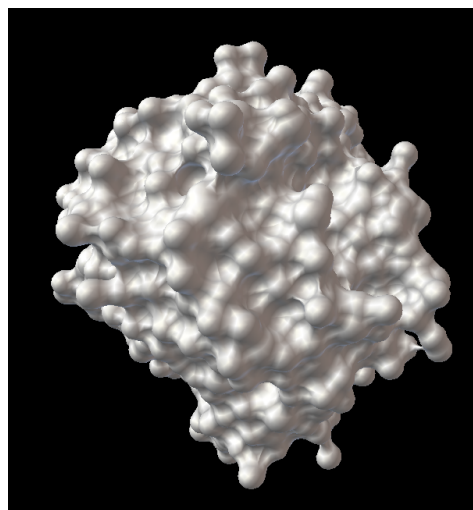
PMV from MGLTools is a powerful molecular viewer that has a number of customizable features and comes with many pluggable commands ranging from displaying molecular surfaces to advanced volume rendering.

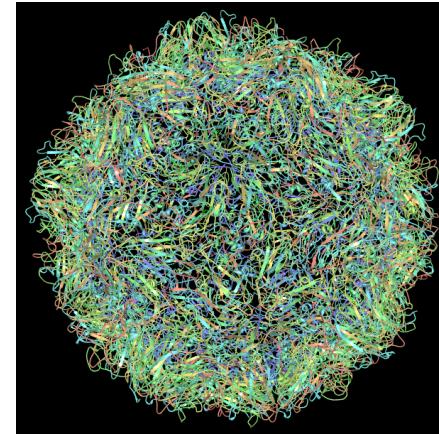## A region of human rhinovirus 1A (HRV-1A)
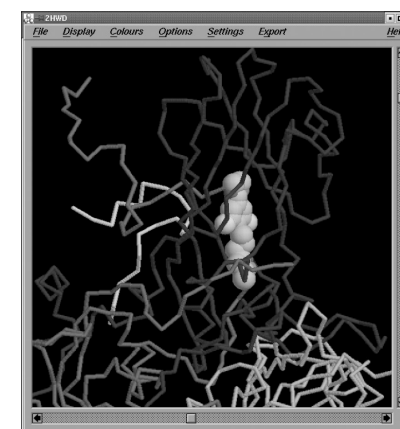
► including a bound drug molecule (PDBid 2HWD).
► The virus proteins are shown as a simple backbone trace, with the drug represented as space-filling spheres.

Human rhinovirus 1a coat protein

Asymmetric Unit
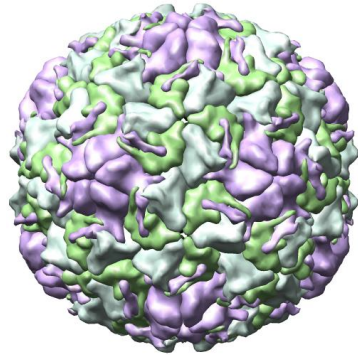
Human rhinovirus 1a coat protein

CATH classification

Domain
 2hwd100

Class
 Mainly Beta

Architecture
 Sandwich

Topology
 Jelly Rolls

## Secondary structure of human thioredoxin (1ERT)

▶ The protein β-strands are represented by arrows from the N- to the C-terminus, and α-helices as spiral ribbons.

▶ Regions without defined secondary structure are shown as a smooth tube.

▶ The four β-strands form a β-sheet at the center of the structure, easily visible in this kind of representation.

▶ Image generated by MolScript and render.

A molecular surface drawn as a mesh.
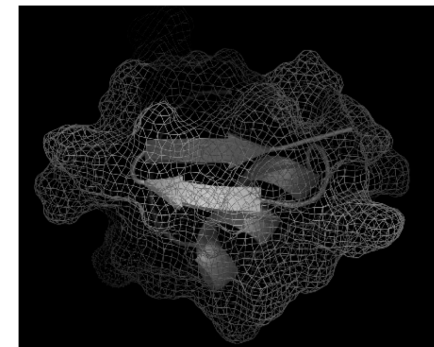
▶ A molecular surface drawn as a mesh,

▶ overlaid on a secondary structure representation of the toxin LQ2 from Leiurus Quinquestriatus (PDBid 1LIR).

▶ image was prepared within PyMol

Structure of c-AMP-Dependent protein kinase (2CPK)
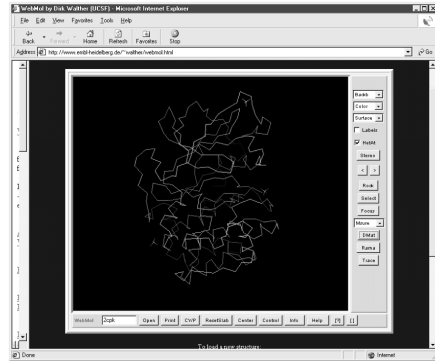
- ▶ displayed using WebMol and MolSurfer (Java)
- ▶ some fairly advanced features:
  1. interactive Ramachandran plot
  2. link of a 2D projection of a macromolecular interface to a 3D view of the structures.

MICE scene interchange format
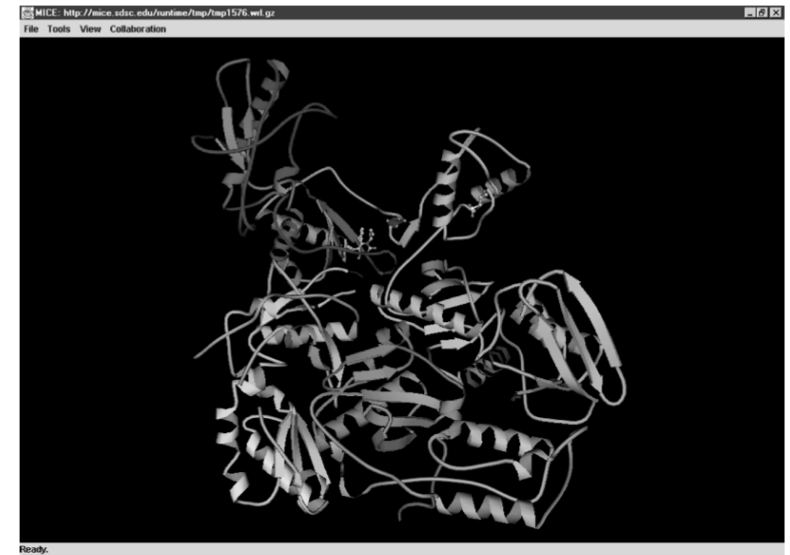
The MICE project is addressing these issues through development of a custom XML-based language.

Need of tools for analyzing, understanding, and exchanging data

The volume of data produced by genome projects, X-ray cristallography, NMR spectroscopy, and electron and confocal microscopy presents the bioinformatics community with new challenges for analyzing, understanding, and exchanging this data

Molecules to Maps: tools for visualization and interaction in support of computational biology
– Eileen T. Kraemer and Thomas E. Ferrin

Frequently, data in scientific computing is in its abstract form a finite point set in space, and it is sometimes useful or required to compute what one might call the "shape" of the set.
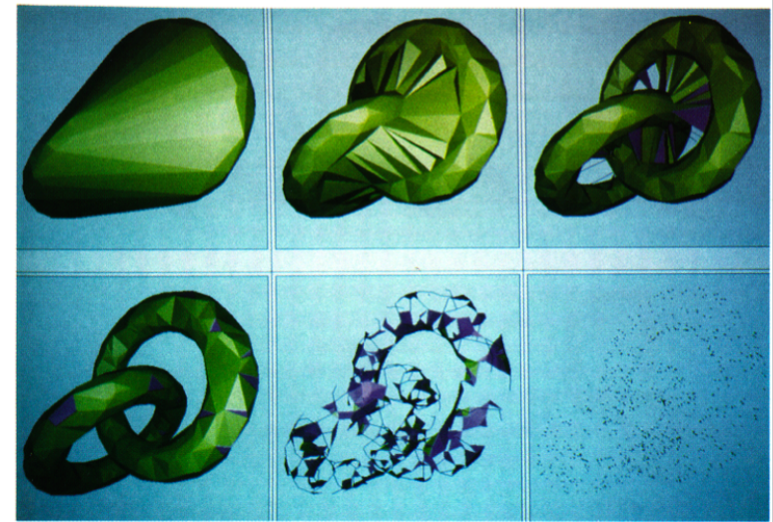
The article

Edelsbrunner, H. and Mücke, E. P. 1994. Three-dimensional alpha shapes. *ACM Trans. Graph.* 13, 1 (Jan. 1994), 43-72. DOI=
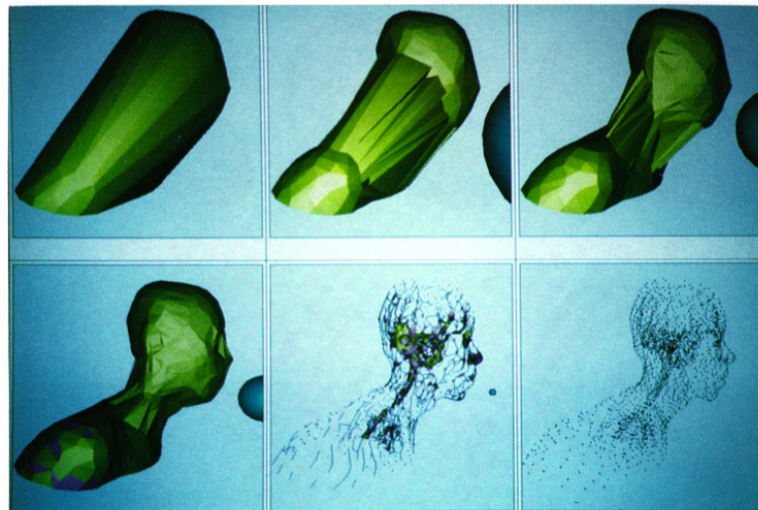http://doi.acm.org/10.1145/174462.156635

introduces the formal notion of the family of α-shapes of a finite point set in R^3.

Each shape is a well-defined polytope, derived from the Delaunay triangulation of the point set, with a parameter $\alpha \in$ R controlling the desired level of detail.
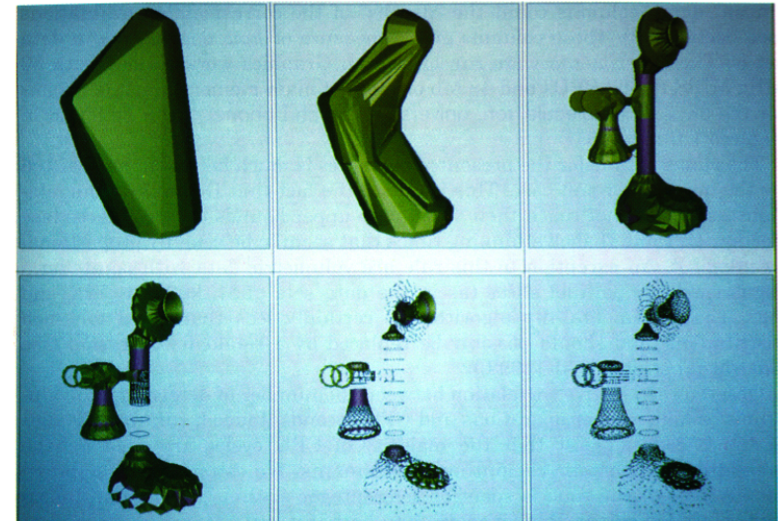
An algorithm is presented that constructs the entire family of shapes for a given set of size n in time O(n^2), *worstcase*.
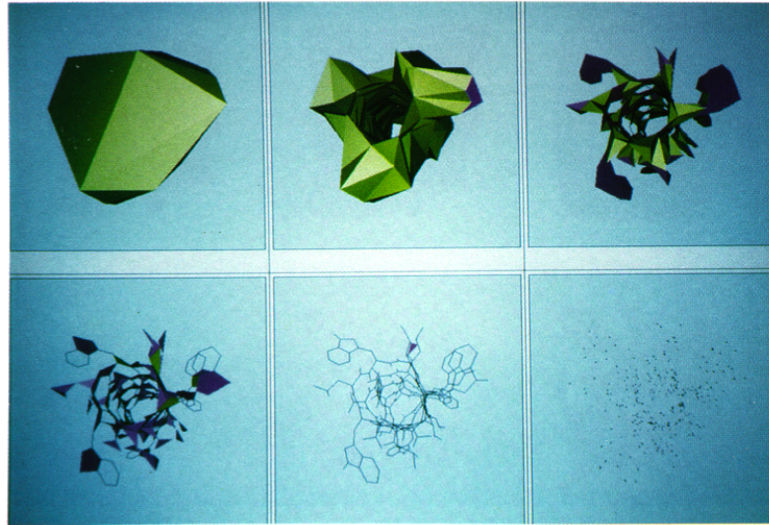
aaaaaaa

aaaaaaa

aaaaaaa