Interactive Visualization of Bio-molecules and their Properties

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Different molecular visualization techniques

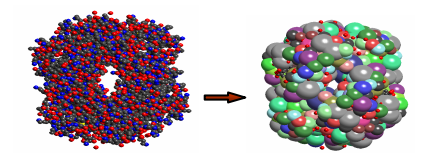
Introduction

Visualizing large bio-molecules in an interactive environment is a key step in understanding the structure and function of complex organic systems. We present a variety of molecular visualization techniques which emphasize high visual quality as well as real-time performance.

In addition to visualization, high-performance techniques for computing essential properties of large bio-molecules is also presented.

Molecular hierarchy

A *level-of-detail* hierarchy is built based on biochemical connectivity and grouping.



Atoms level, rendered by atom colors — Residues level, rendered by residue colors

Hemoglobin molecule (1A00.pdb), *union of balls* rendering

Volume rendering

We use 3D texture based hardware accelerated volume rendering to render the molecules with transparency.

The new RawV volume format developed at CCV supports vector valued volume representation.

Isocontouring

Volumetric functions including electron density, electrostatic potential, hydrophobicities etc. yield isocontours which approximate surfaces like the solvent accessible surfaces which can be visualized.

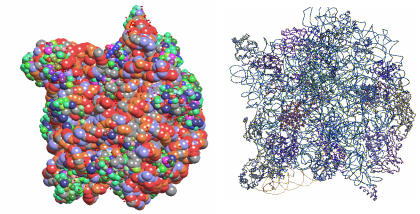
The MAChE Data set, provided by Prof N Baker, (Washington University, St Louis) and meshed by Y Zhang. The adaptive meshing shows the narrow gorge on the surface. The mesh is rendered using the hydrophobicity function.

Image based rendering

To rapidly visualize the ball-and-stick model, we use texture-mapped quadrilaterals, known as impostors, to represent:

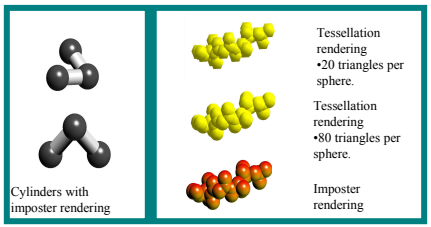
- displacement,
- normal, and
- transparency

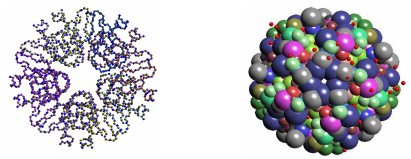
Both spheres and cylinders can be represented with impostors, which obviates the need for tessellation and reduces the complexity of the geometry sent to the graphics card.



Residue level union of balls rendering — Backbone chains

The large ribosomal subunit (1JJ2.pdb)





The Backbone of the molecule is rendered using alternating spheres and cylinders, each rendered using single quads with full lighting.

Residues rendered with residue coloring. Each residue was obtained as a union sphere containing all the atoms within the residue.

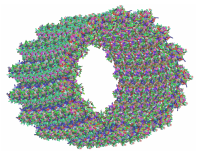
Trypsin inhibitor (1BHC.pdb)

Correct per pixel lighting is implemented in the fragment shaders to obtain high quality images. Interactive updates of like color, light source properties etc. are possible.

Functions and properties of the molecules

The 1.2 million microtubule

This is the largest biomolecule we have tested our imposter model on. It contains 1.2 million atoms, each rendered with diffuse and specular highlights as spheres. We obtained around 5 frames per second on a desktop with a Nvidia GeForce 4 graphics card.

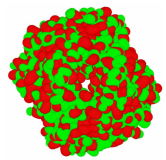


Microtubule, dataset generated by Prof D Sept, Department of Biomedical Engineering, Washington University, St Louis.

Volume functions

In the case of a gaussian blurring of the atoms to approximate the electron density, we can define the function f as :

$$f(x, y, z) = 0 = \text{sum} (e^{(\text{blobby}*r/ri - \text{blobby})}) - I$$



Hemoglobin (1A00.pdb), Hydrophobicity Volume Rendering
Green represents hydrophobic regions. Values generated by L Kapcha and Prof P Rossky (Director, Institute for Theoretical Chemistry, Univ Texas at Austin)

The hydrophobicity of a molecule can also be represented in volumetric format by a gaussian around the atom centers.

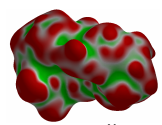
Differential properties

The two main curvatures in differential geometry are

- ***Mean curvature*** **H** and
- ***Gaussian curvature*** **K**.

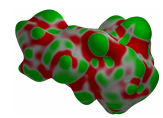
Let k_{min} and k_{max} be the minimum and maximum curvatures at the point. Then,

$$\mathbf{H} = 1/2 (k_{min} + k_{max}) \quad \text{and} \quad \mathbf{K} = k_{min} k_{max}$$



Mean curvature

red white green
-0.1 0 1.0



Gaussian curvature

red white green
-0.01 0 0.01

Protein Kinase From Rat (1A06.pdb)

Let f (x,y,z) = 0 represent an implicit function in $\mathbf{R}^3$. The curvatures H and K can be evaluated as

$$H = (C (f_x^2 (f_{yy} + f_{zz})) - 2 * C (f_x f_y f_{xy})) / (2 * (C (f_x^2))^{1.5})$$

$$K = (2 * C (f_x f_y (f_{xz} f_{yz} - f_{xy} f_{zz}))) / ((C (f_x^2))^2)$$

Where C represents a cyclic summation over x, y and z, and the subscripts denote partial differentiation with respect to those variables.

Integral properties

- Volume occupied by the molecule, defined by the solvent accessible surface or the solvent excluded surface.
- Exposed area

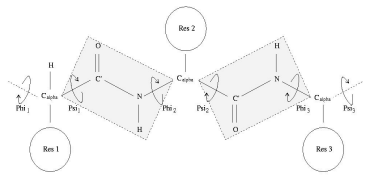
The *Contour Spectrum*, a general program for calculating such properties over volumetric data also visualizes the results for all isovalues.

Flexibility modeling

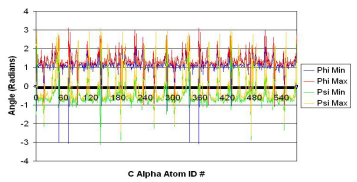
The backbone of a protein chain consists of the repeating subunit:

$$(\ldots - N - C_{alpha} - C' - \ldots)$$

The rotation around the ($N - C_{alpha}$) and ($C_{alpha} - C'$) bonds are the Phi and Psi torsion angles, respectively. A protein's flexibility is based in large part on its entire set of Phi and Psi angles.



Phi / Psi Angles for C Alpha Atoms in Goodsell



Datasets generated by D Goodsell, Scripps Research Institute