Virtual Reality Modeling for Structural Biology

Jürgen Sühnel (jsuehnel@imb−jena.de)
Institut für Molekulare Biotechnologie, Postfach 100813, D−07708 Jena / Germany

Introduction

Visualization plays a central role in understanding biopolymer structures. The usual visualization method is to retrieve the coordinate files from a structure database and then to use one of the molecular graphics software packages. On the other hand, one would often prefer to have biopolymer images directly available without the need to spend some time for visualization or even without having access to a molecular graphics software. This is especially important for the large and heterogenous community outside structural biology.
The recent developments in the World−Wide Web enable one very easily to transfer images or videos over the Internet. We have, therefore, started in 1993 to set up an Internet−based

Image Library of Biological Macromolecules (http://www.imb−jena.de/IMAGE.html).

Currently, the Library contains more than 3500 images of about 300 structures. The images are in the public domain and can freely be retrieved from the IMB Jena WWW server.

In 1995 the new VRML format was defined. The Virtual Reality Modeling Language (VRML) is essentially a three−dimensional image format supplemented by network tools. Contrary to the static images it enables one to interact with the three−dimensional image objects. Of course, for biopolymers this can be done much better using molecular graphics packages. On the other hand, VRML viewers are already becoming standard parts of current web browsers. Insofar it is immediately obvious that this new tool is of relevance for structural biology.
We have therefore extended the Image Library by a Virtual Reality Division. Besides the pioneering work done at the Imperial College London and at the Technical University of Darmstadt, this was one of the first VRML applications in biology and to the best of our knowledge the very first application which was not devoted to demonstration purposes alone. The VRML division contains now already about 650 VRML representations of biopolymer structures.

[1] Sühnel, J., Image Library of Biological Macromolecules, Comput. Appl. Biosci. 1996, 12, 227−229.

What is VRML ?

The Virtual Reality Modeling Language (VRML) is a standard for describing interactive three−dimensional scenes delivered across the Internet. VRML is a subset of the Open Inventor ASCII file format and it describes 3D objects or scenarios in an object oriented manner. The basic elements are various node types: shape nodes (points, lines, spheres, cylinders,...) property nodes (color, texture maps, geometry transformation,...) group nodes (for implementing a hierarchical structure), camera nodes, light nodes, WWWInline nodes (for loading other VRML files into the current scene) and WWWAnchor nodes (hyperlinks). The VRML 1.0 specification was finalized in May 1995 and the VRML 2.0 specification is currently under development.

How to create VRML representations ?

We have generated the VRML files of biopolymers and of the corresponding building blocks (amino acids, nucleotides) using InsightII from Molecular Simulations, the MIDASPLUS molecular graphics and display system and the SGI Iris Explorer EyeChem modules written by Omer Casher, Imperial College, London. InsightII has a direct VRML interface, whereas in the other two cases, first files in the Inventor format have to be created which then have to be converted to the VRML format.

We would like to encourage developers of other molecular graphics packages to include VRML interfaces into their software tools.

More recent examples are the WebLab viewer (Molecular Simulations), the Tripos Molecular Inventor Netscape Navigator Plugin and the object−oriented three−dimensional visualization development kit Molecular Inventor (Slicon Graphics), which all can generate either Inventor or VRML files.

According to our experience the best current tool for creating VRML files is InsightII.

How to view VRML files ?

For visualizing VRML files one needs VRML viewers. The first generally available VRML viewer was
WebSpace
from Silicon Graphics. It was released for the first platforms in May 1995. The claim that VRML viewers will become standard parts of future web browsers is confirmed by the VRML plugins of
Netscape Navigator Gold
and of the Microsoft
Internet Eplorer 3.0. Especially interesting for structural biology is the viewer
i3D
developed at CERN. It seems to be the first viewer which supports crystal eyes stereo representations.
CosmoPlayer
(Silicon Graphics) is one of the first viewers which supports the upcoming VRML 2.0 specification. A comprehensive collection can be found in the VRML repository at the San Diego Supercomputer Center.

Further usage of VRML files

The VRML format is appropriate for further annotation with any types of notes using, for example IRIS Annotator or Showcase, for Media Mail or for real time collaboration with InPerson. VRML files can be combined with Java scripts

Structural Biology web sites

Crystal packing visualization for PDB files: Protein Crystallography Group,University of British Columbia (http://laue.biochem.ubc.ca:8080/cgi−bin/ssis/banff/xpack.html)

Chemical Examples of VRML: Dep. of Chemistry, Imperial College, London (http://www.ch.ic.ac.uk/VRML/)

VRML in Chemistry: Instutut für Physikalische Chemie, TH Darmstadt (http://ws05.pc.chemie.th−darmstadt.de/vrml/)

Protein Motions Database: Stanford University Medical Center (http://hyper.stanford.edu/~mbg/ProtMotDB/vrml/)

Interactive Membrane Builder: Physical and Theoretical Chemistry, University of Oxford (http://bellatrix.pcl.ox.ac.uk/people/alan/WebSpace/builder/form.html)

Image Library of Biological Macromolecules: Biocomputing Group, IMB Jena (http://www.imb−jena.de/IMAGE.html)

The Virtual Reality Division of the Image Library of Biological Macromolecules

imb JENA

Image Library
of
Biological Macromolecules

Virtual Reality Division

Note, that for all of the following structures an annotation file, color coded distance plots and more (static) images including stereo representations are available in the original non-VRML part of the IMAGE LIBRARY.

- **Introduction**
- **Building Blocks (VRML)**
  - Amino Acids
  - Nucleotides and Basepairs
- **Macromolecule Structures (VRML)**
  - PROTEINS
  - RNA (including RNA-protein complexes and DNA-RNA hybrids)
  - DNA (including DNA-protein complexes)
  - CARBOHYDRATES
- **Other Chemistry/Biology VRML sites**
  - Crystal Packing Visualization by VRML (for PDB files) *(Protein Crystallography Group at the University of British Columbia)*
  - Chemical Examples of VRML *(Department of Chemistry, Imperial College, London)*
  - VRML in Chemistry *(Institut für Physikalische Chemie, TH Darmstadt)*
  - Atomic orbitals *(Chemistry Department, Virginia Tech)*
  - MathMol Library of 3-D Molecular Structures *(New York University, Scientific Visualization Department)*
  - Protein Motions Database *(Stanford University Medical Center)*

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J. Sühnel, (e-mail: jsuehnel@imb-jena.de) - Biology and Computers
Biocomputing Group, **Institut für Molekulare Biotechnologie**, POB 100 813, D-07708 Jena / Germany

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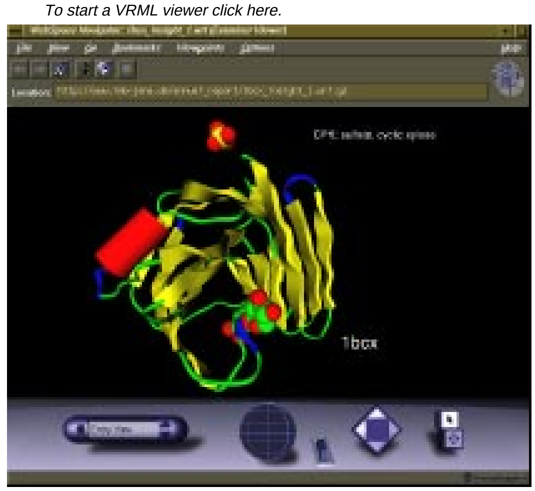
Secondary structure representation of the Bacillus circulans xylanase complexed with sulfate and cyclic xylose
(PDB code − 1bcx;
Wakarchuk et al., Protein Sci. 1994, 3, 467−475;
helix − red, sheet − yellow, turn − blue)
To see a better quality image click here.
To start a VRML viewer click here.



Problems

VRML browsers still suffer from various problems. For example, complex structures in high−quality representations may yield very large datasets. Fortunately the compression rate is rather high, in many cases 90%. This reduces the bandwidth required. On the other hand, uncompression takes time. Therefore, it may happen that currently less powerful computers are not able to manage larger VRML files. You will come across such examples if you check out the Virtual Reality Division of the Image Library. One should realize, however, that the performance of the viewers, like WebSpace for example, has already dramatically increased since May 1995.

Outlook

The new VRML format has already a lot to offer for a better dissemination of structural information on biopolymers. One interesting application we expect in the near future is that online journals will include VRML images.

How a VRML file looks like (ball and stick representation of alanine)

```
#VRML V1.0 ascii

Separator {
  Material {
  ambientColor    0.1 0.1 0.1
  diffuseColor    1 1 1
  specularColor   0.9 0.9 0.9
  shininess       0.8
  }
  PerspectiveCamera {
  position        1.634 0.172 39.57
  orientation     0 0 1  0
  focalDistance   36.37
  heightAngle     0.360261
  }
  Separator {
  Transform {
    translation   2.553 0.243 3.632
    rotation      −0.565042 0 0.825062  1.954
  }
  Material {
    diffuseColor  0 0.364 1
  }
  Cylinder {
    parts         SIDES
    radius        0.18
    height        0.73
  }
  }
  Separator {
  Transform {
    translation   1.993 −0.029 3.249
    rotation      −0.565042 0 0.825062  1.954
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.18
    height        0.73
  }
  }
  Separator {
  Transform {
    translation   2.884 0.645 3.832
    rotation      0.161967 0 −0.986796  0.195
  }
  Material {
    diffuseColor  0 0.364 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.54
  }
  }
  Separator {
  Transform {
    translation   2.987 1.175 3.849
    rotation      0.161967 0 −0.986796  0.195
  }
  Material {
    diffuseColor  1 1 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.54
  }
  }
  Separator {
  Transform {
    translation   3 0.222 3.964
    rotation      0.64509 0 −0.764107  2.195
  }
  Material {
    diffuseColor  0 0.364 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.54
  }
  }
  Separator {
  Transform {
    translation   3.335 −0.093 4.247
    rotation      0.64509 0 −0.764107  2.195
  }
  Material {
    diffuseColor  1 1 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.54
  }
  }
  Separator {
  Transform {
    translation   1.28 −0.576 3.543
    rotation      0.744089 0 0.66808  2.133
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.18
    height        1.538
  }
  }
  Separator {
  Transform {
    translation   1.329 0.384 2.712
    rotation      −0.66808 0 0.744089  0.756
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.18
    height        1.51
  }
  }
  Separator {
  Transform {
    translation   1.814 −0.332 2.861
    rotation      −0.890597 0 −0.454794  2.216
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.553
  }
  }
  Separator {
  Transform {
    translation   2.016 −0.665 2.468
    rotation      −0.890597 0 −0.454794  2.216
  }
  Material {
    diffuseColor  1 1 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.553
  }
  }
  Separator {
  Transform {
    translation   1.025 1.23 2.39
    rotation      0.279078 0 −0.960268  0.279
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.15
    height        0.618
  }
  }
  Separator {
  Transform {
    translation   1.188 1.825 2.437
    rotation      0.279078 0 −0.960268  0.279
  }
  Material {
    diffuseColor  1 0 0
  }
  Cylinder {
    parts         SIDES
    radius        0.15
    height        0.618
  }
  }
  Separator {
  Transform {
    translation   0.729 0.853 2.217
    rotation      −0.572119 0 0.820171  1.868
  }
  Material {
    diffuseColor  0 1 0
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.545
  }
  }
  Separator {
  Transform {
    translation   0.302 0.694 1.919
    rotation      −0.572119 0 0.820171  1.868
  }
  Material {
    diffuseColor  1 1 1
  }
  Cylinder {
    parts         SIDES
    radius        0.1
    height        0.545
  }
  }
  Separator {
  Transform {
    translation   0.63 −1.102 3.898
    rotation      −0.511994 0 0.858989  2.005
  }
.
.
.
  Material {
    diffuseColor  1 1 1
  }
  Sphere {
    radius        0.2
  }
  }
  Separator {
  Transform {
    translation   −0.017 −1.451 3.513
  }
  Material {
    diffuseColor  1 1 1
  }
  Sphere {
    radius        0.2
  }
  }
  Separator {
  Transform {
    translation   1.416 −1.811 4.495
  }
  Material {
    diffuseColor  1 1 1
  }
  Sphere {
    radius        0.2
  }
  }
  Separator {
  Transform {
    translation   0.438 −0.366 4.849
  }
  Material {
    diffuseColor  1 1 1
  }
  Sphere {
    radius        0.2
  }
  }
}
```