Visualizing Chemical Data in the Internet
Data-driven and Interactive Graphics

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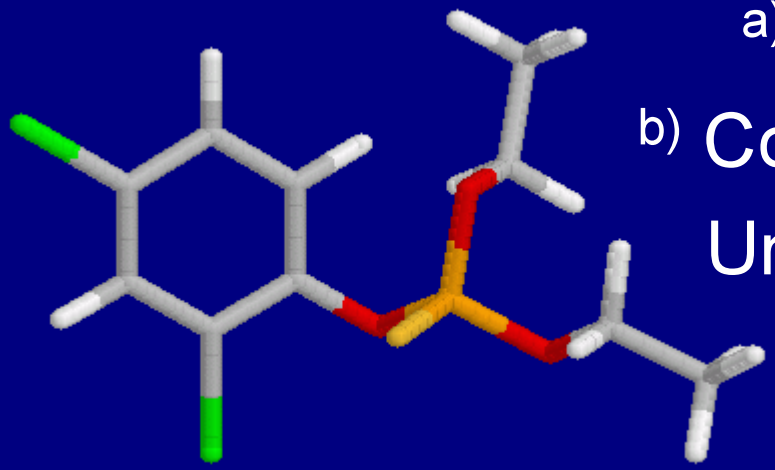
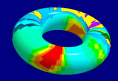
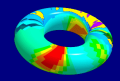




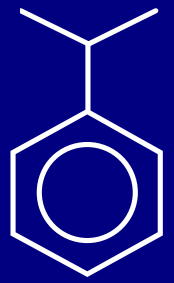
Structure of the Talk

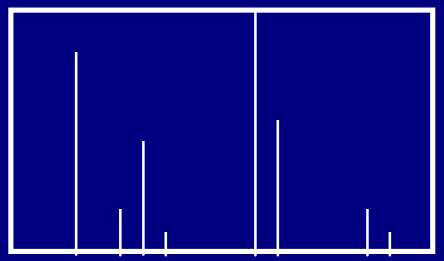
- Chemical information and digital documents
- Molecule representations
- Beyond the simple structure
- Demonstration of progressive isosurface rendering

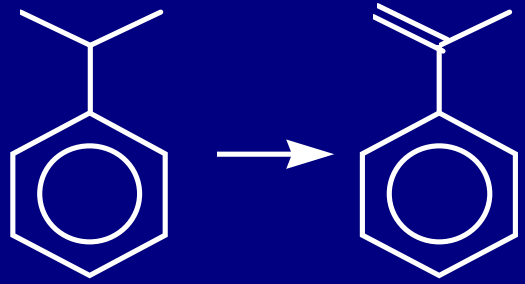


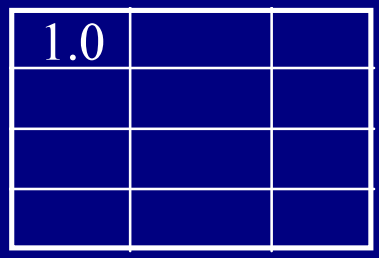
Chemical Information

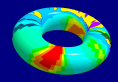
Just a few basic data objects







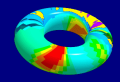




Chemical Information

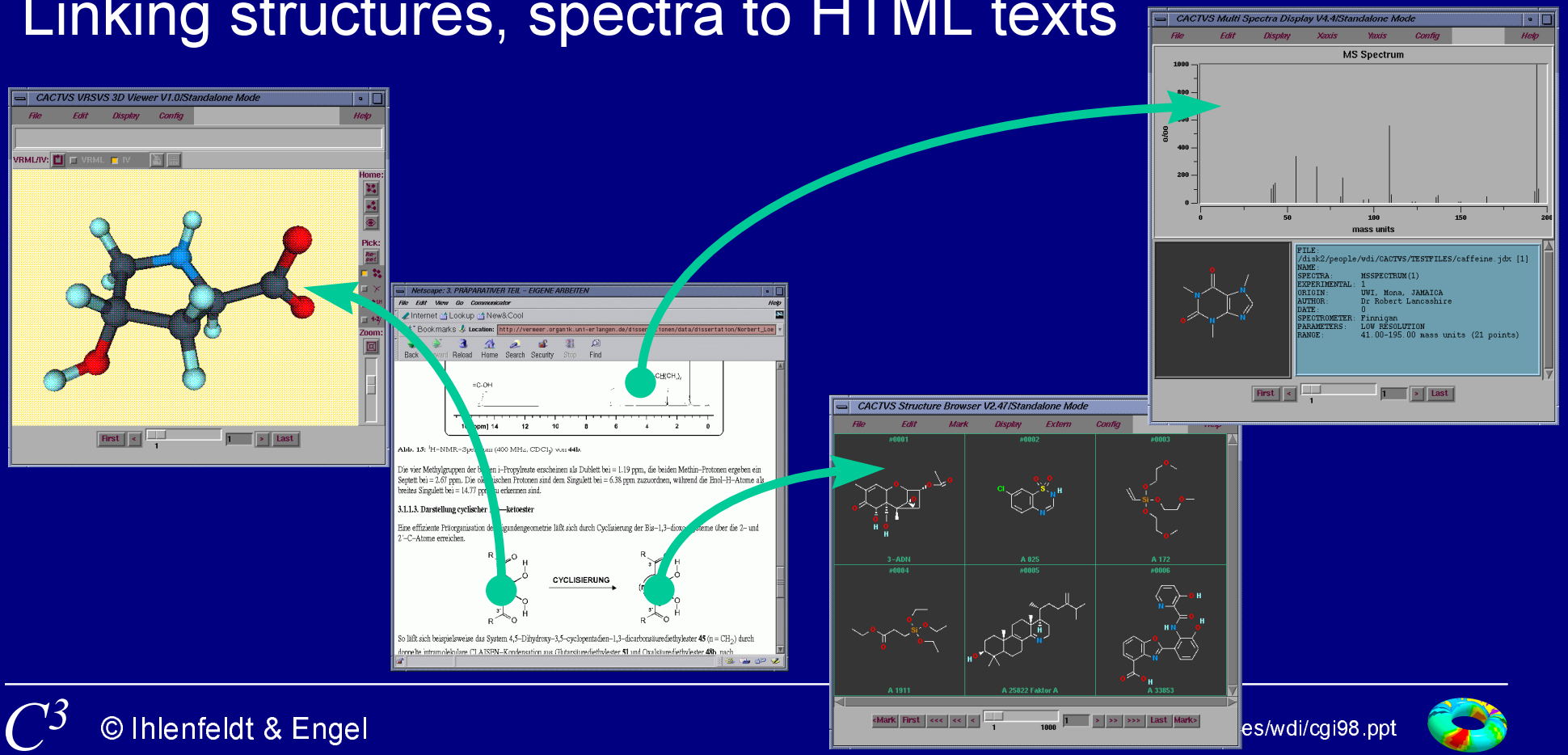
Exchange of data

- about 10 important established exchange formats, plus ca. 30-40 others
- often antiquated design
- chemical MIME types:
- *chemical/x-pdb, chemical/x-mdl-molfile*



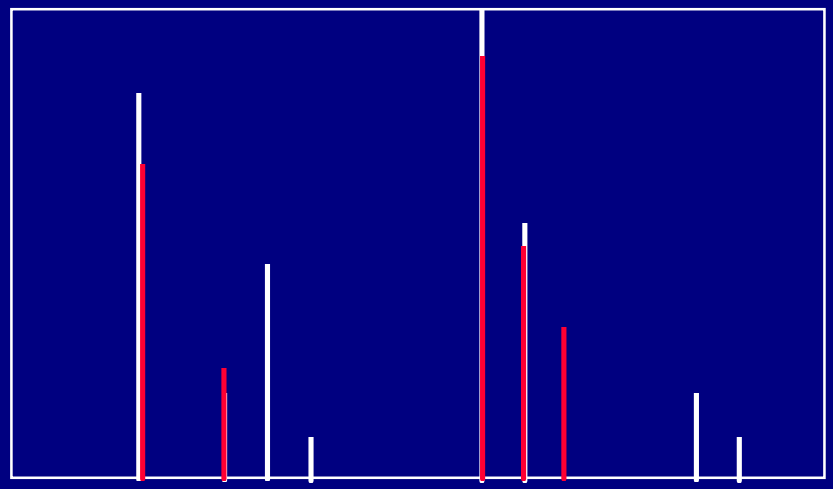
Chemical Information

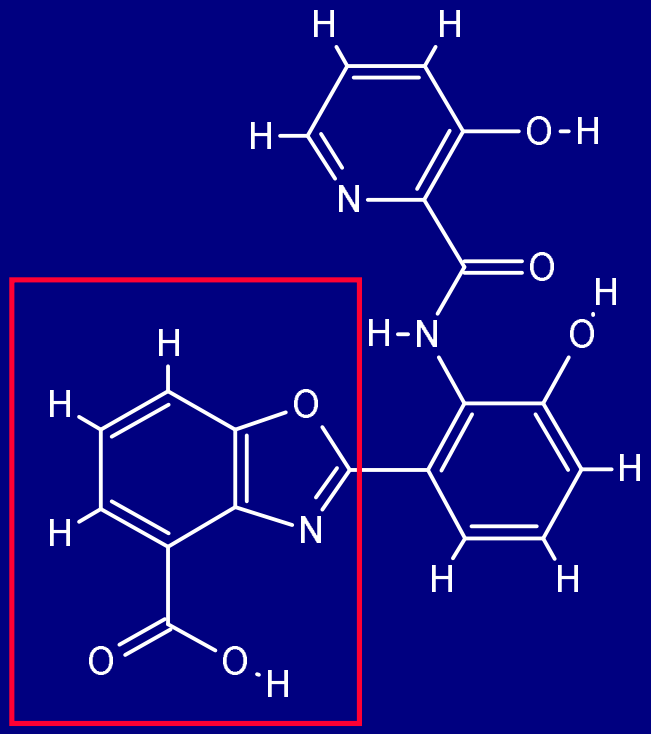
Linking structures, spectra to HTML texts



Chemical Information

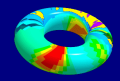
Structure- and property-based non-textual indexing





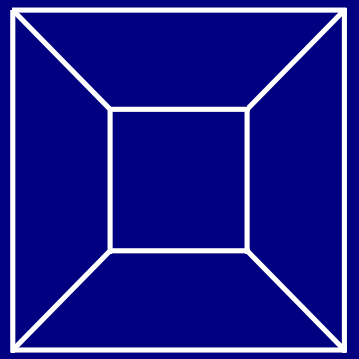
Structure of the Talk

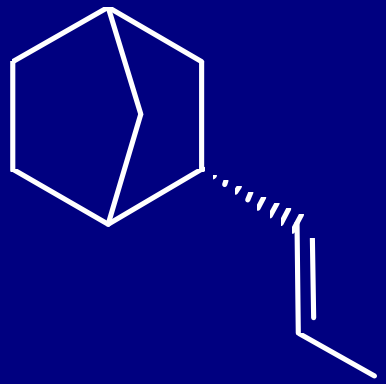
- Chemical information and digital documents
- Molecule representations
- Beyond the simple structure
- Demonstration of progressive isosurface rendering

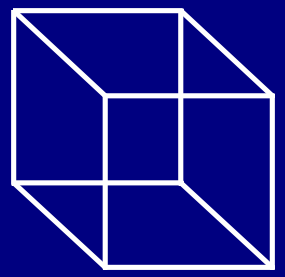


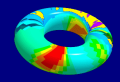
Molecule Representation

2D structure plots - a difficult problem for automatic generation



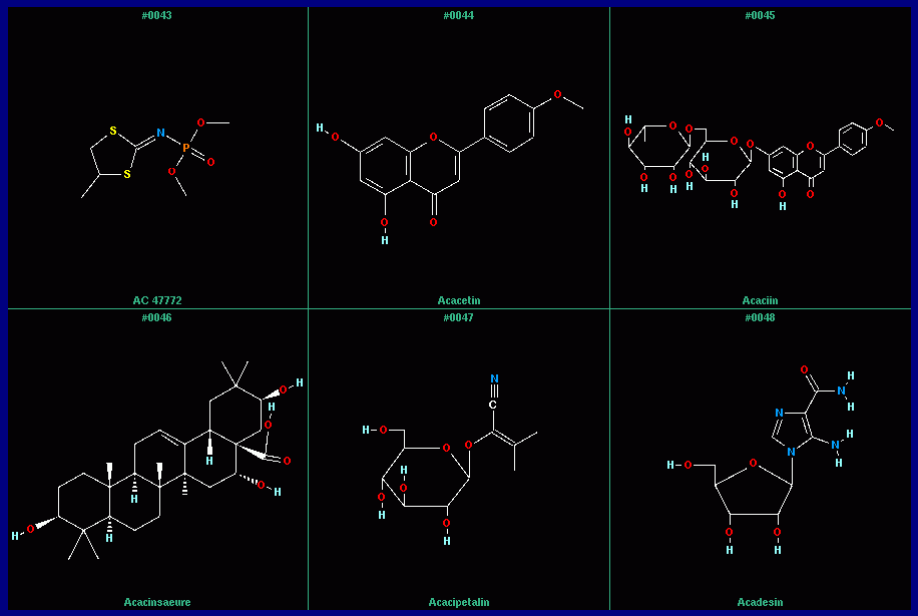


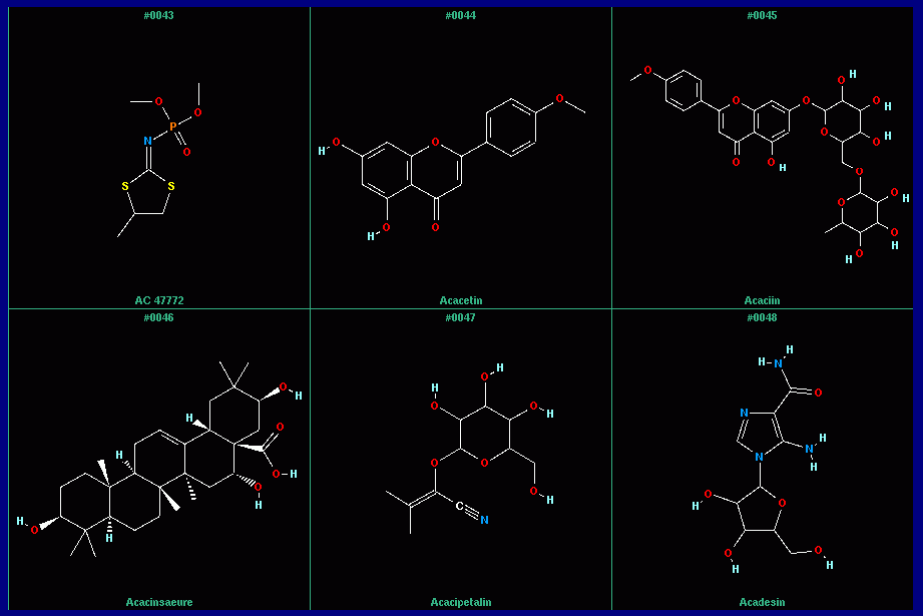




Molecule Representation

Sample recalculated 2D plots

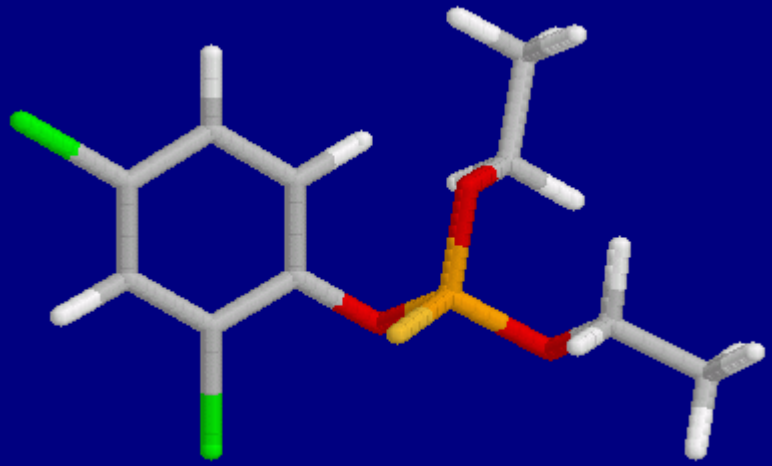


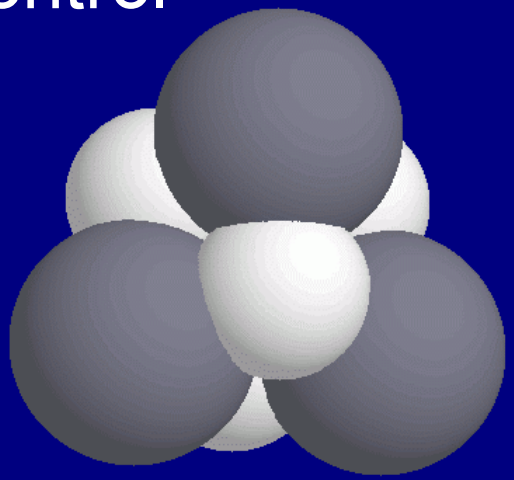


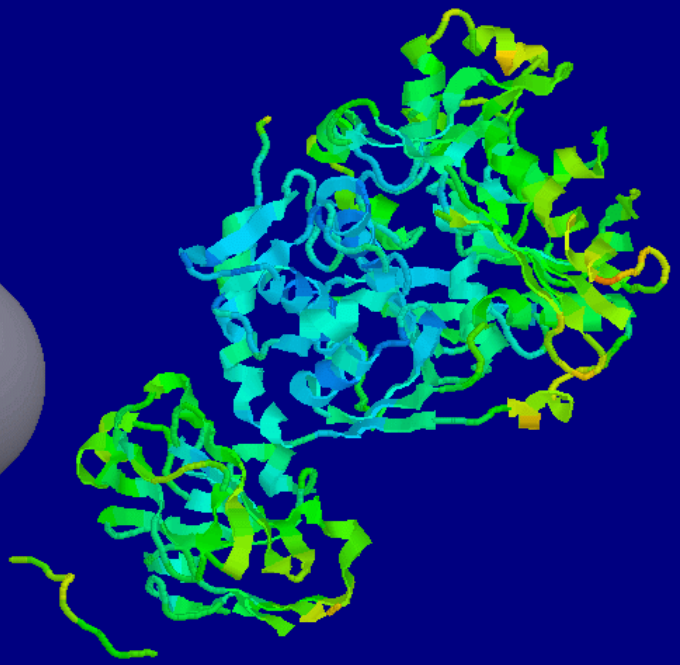
Molecule Representation

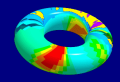
Simple 3D models, on atomic or abstract level

Limited appearance control



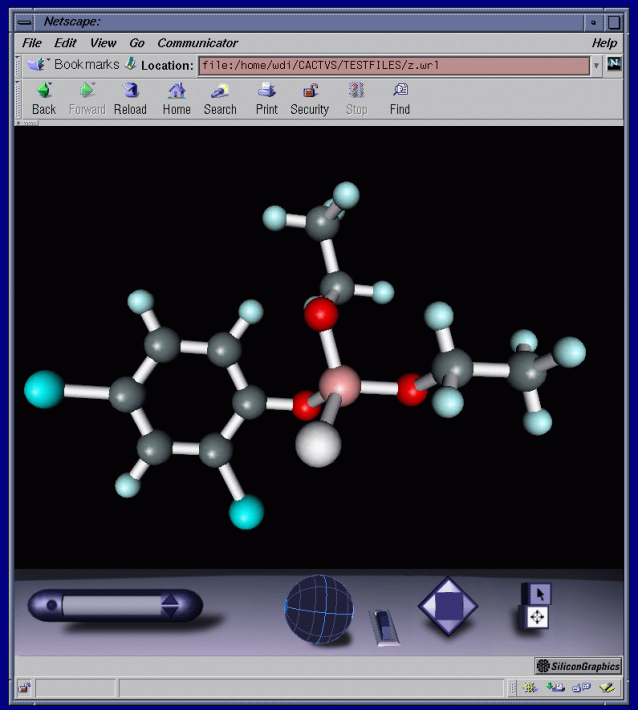


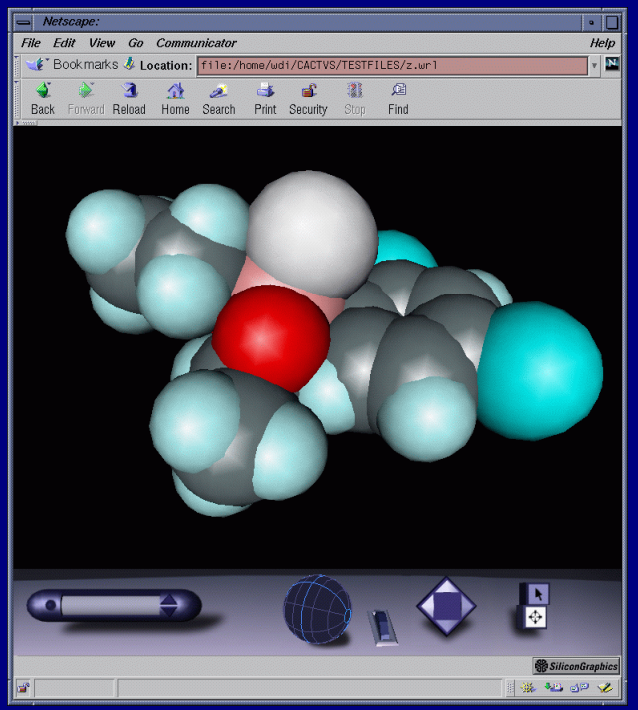




Molecule Representation

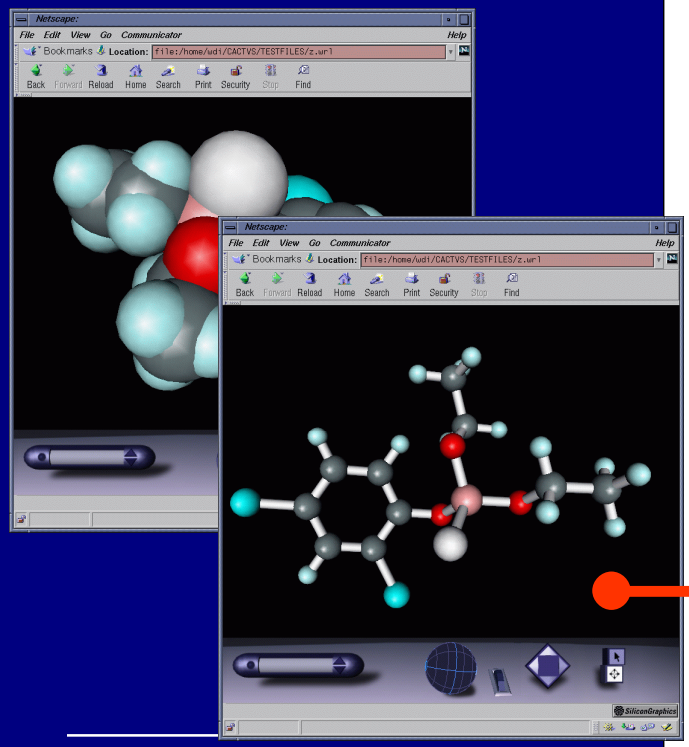
Of course we can use VRML for that...

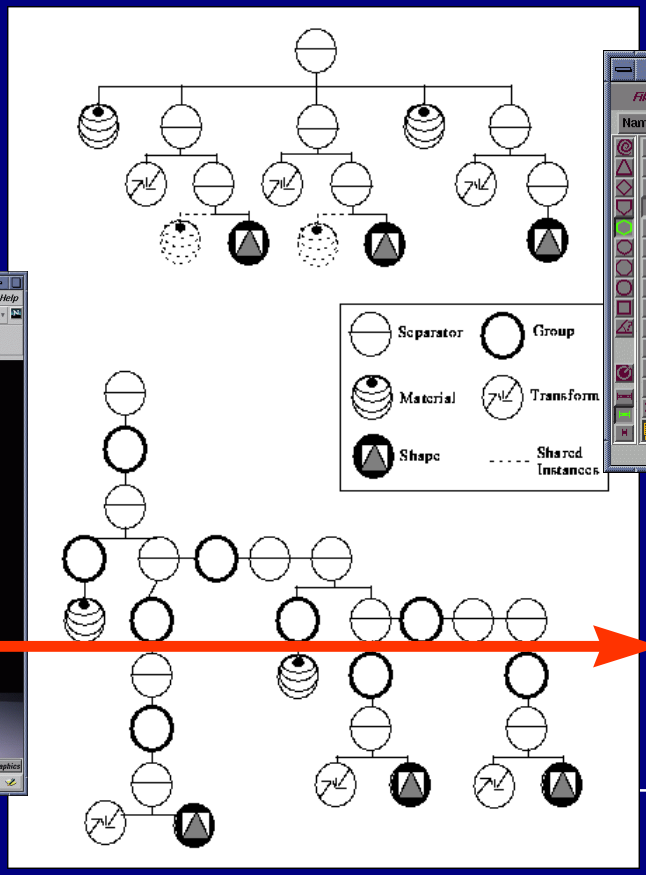


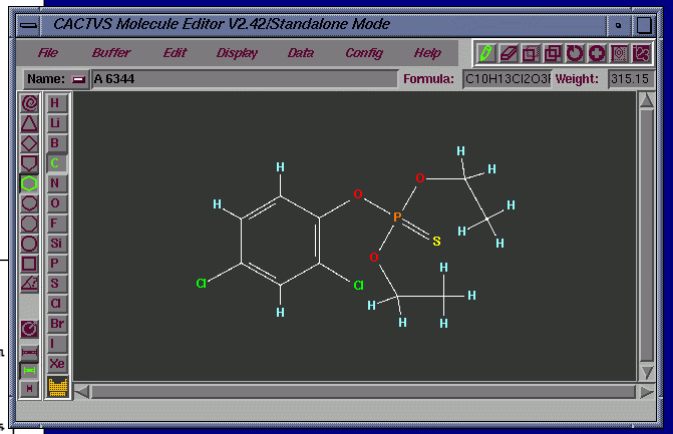


Molecule Representation

... but how do we get the structure back?



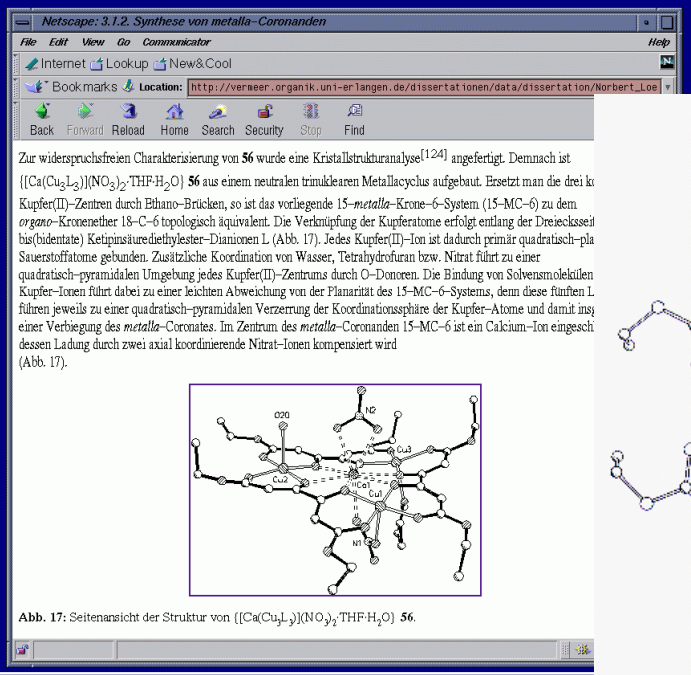


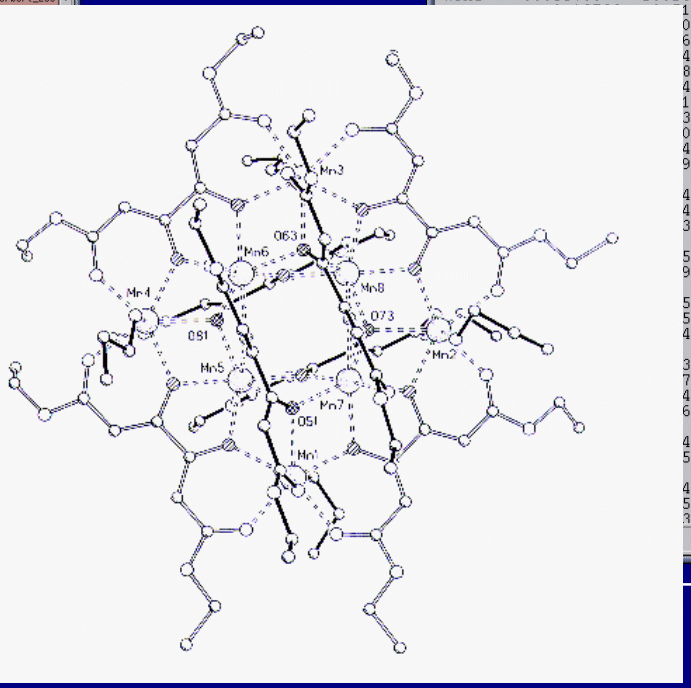


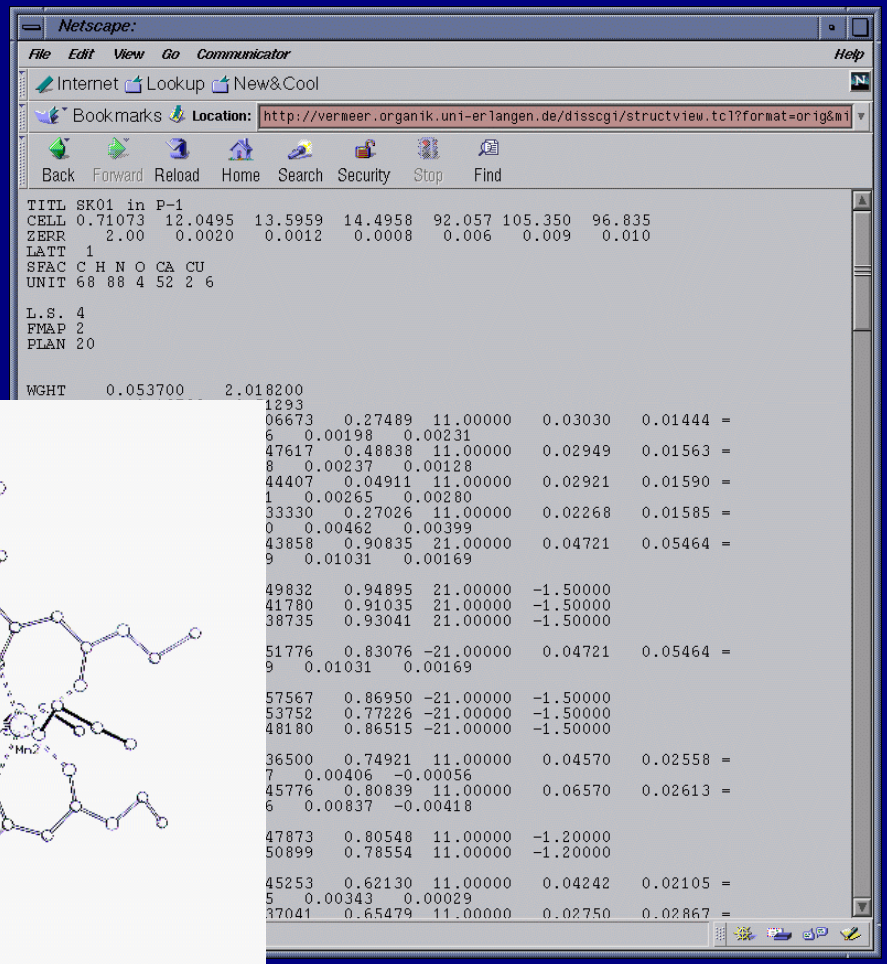
VRML scene analysis with expert system has been demonstrated

Molecule Representation

Conversion on demand from raw data for the true experts…

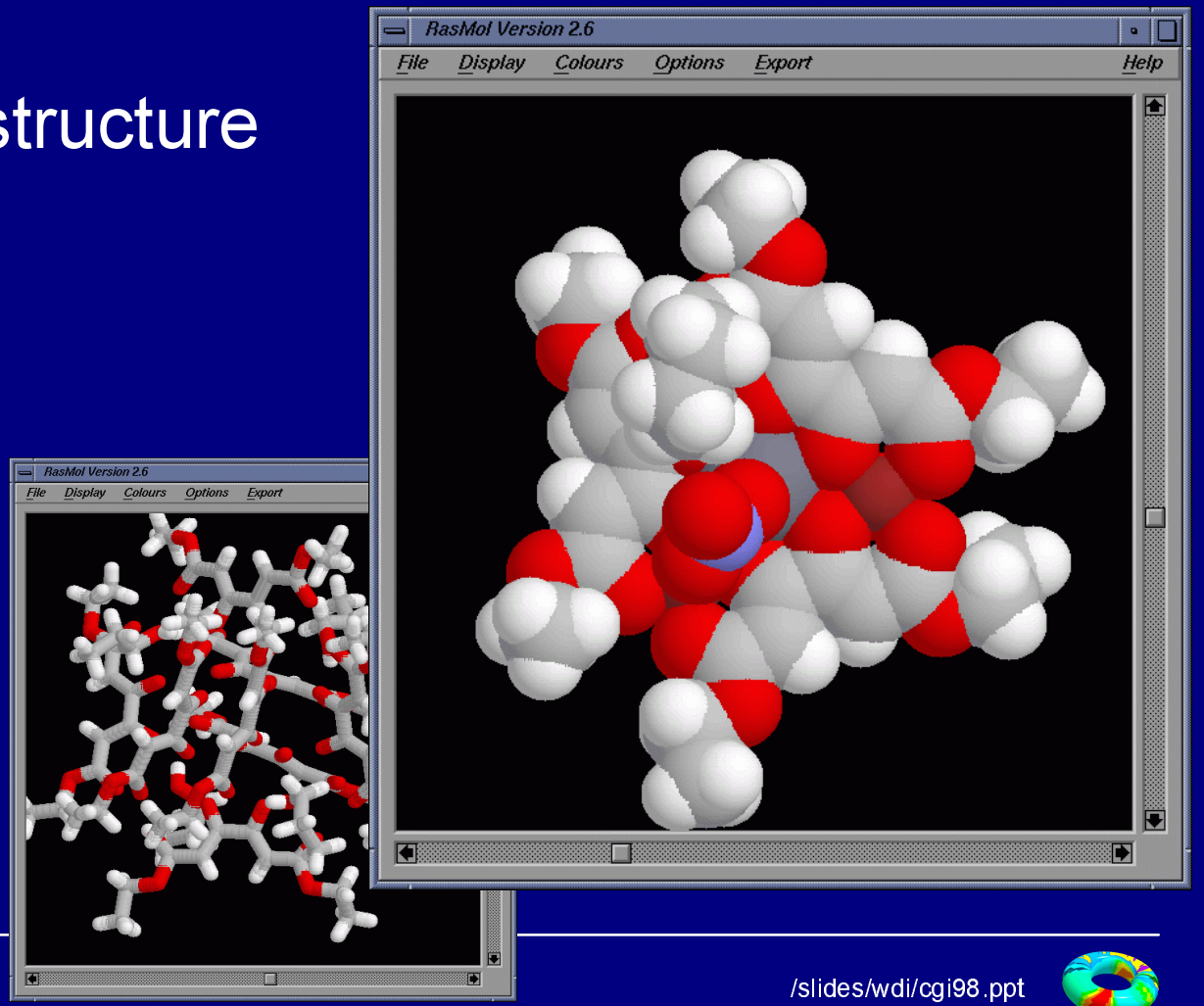






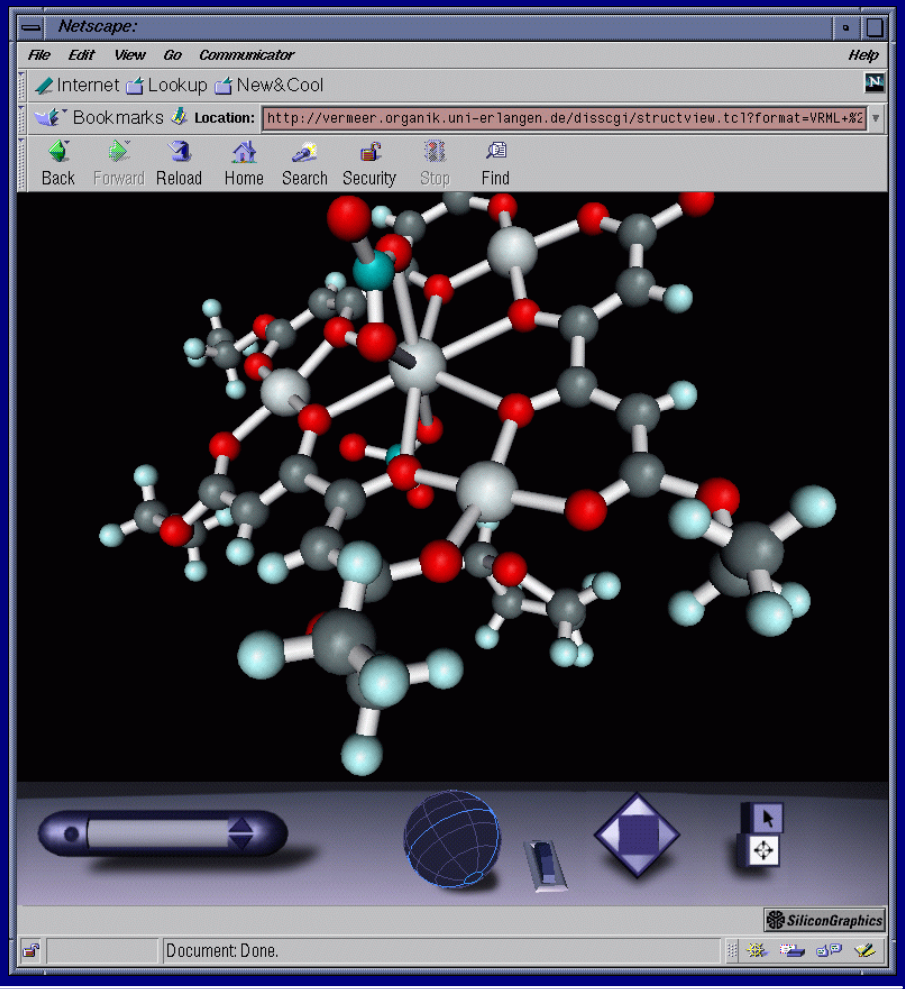
Molecule Representation

... via field-specific structure exchange formats, requiring special viewer software ...



Molecule Representation

... to the form for the casual student user equipped with a standard VRML browser



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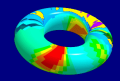
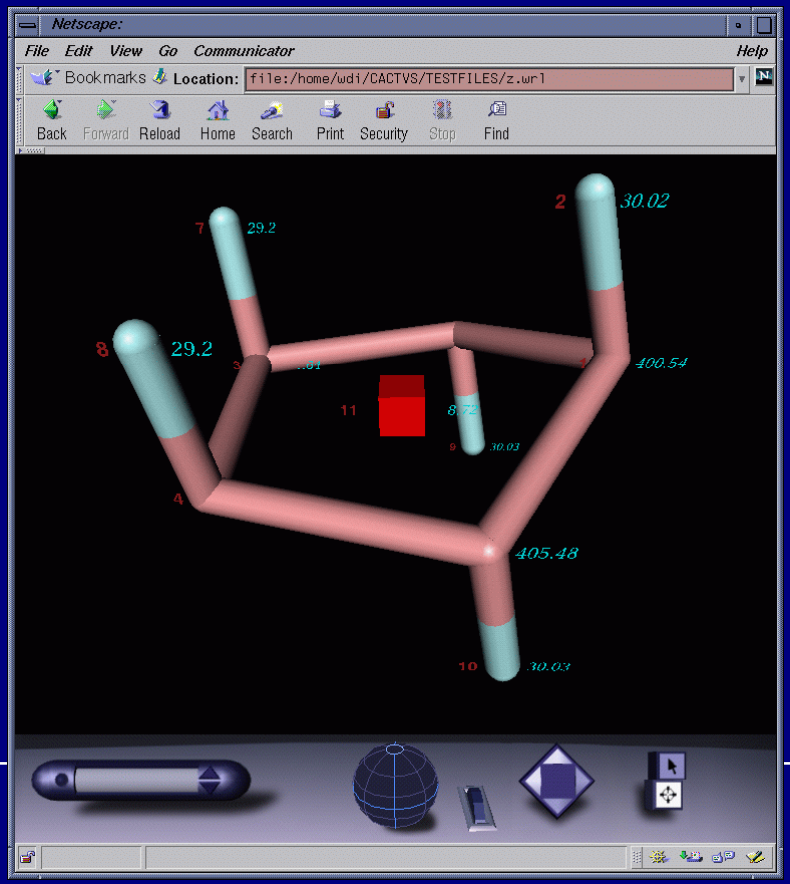
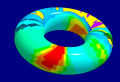


Beyond the Simple Structure Model

Computing expensive properties at critical 3D points

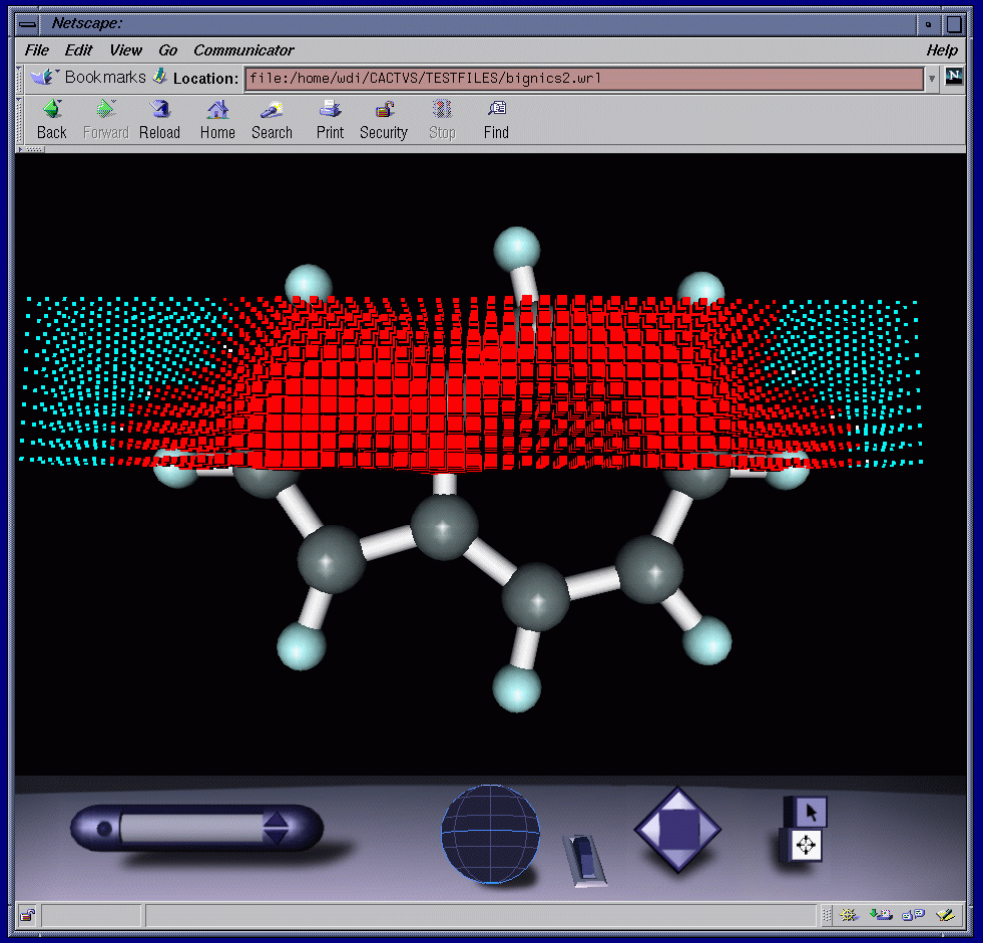




Beyond the Simple Structure Model

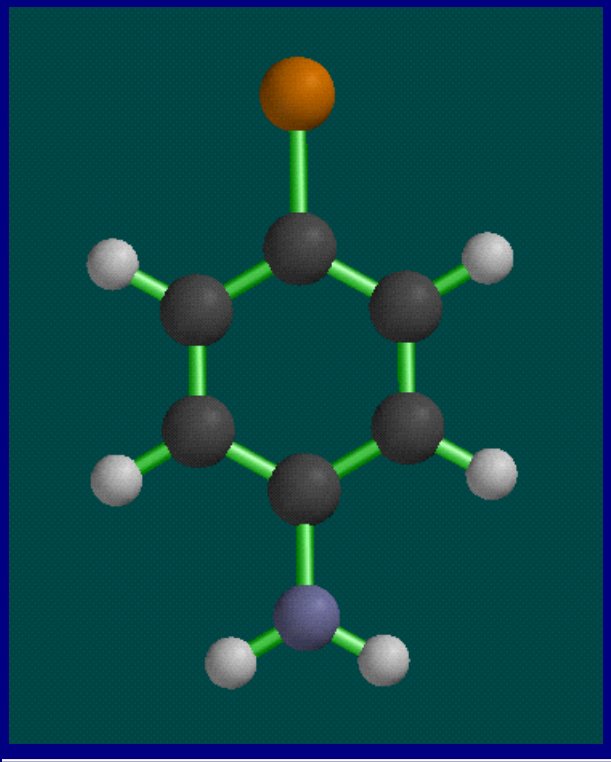
More computations on a coarse grid

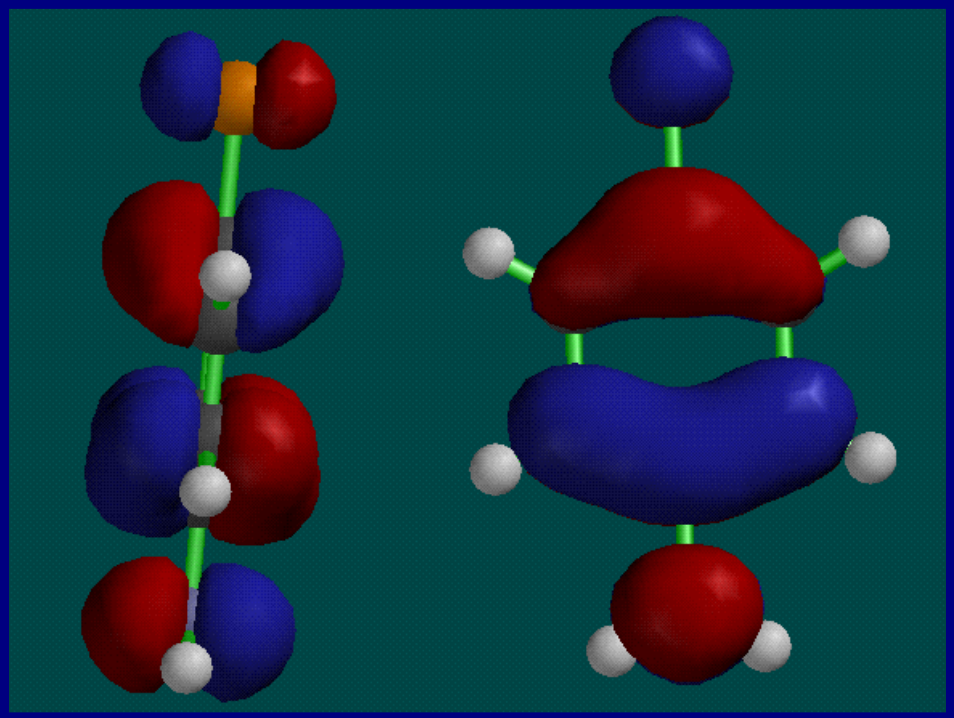
Isotropic Component of NMR ^{31}P Shielding Tensor



Beyond the Simple Structure Model

Molecular orbitals - typical volume data sets





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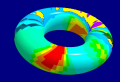
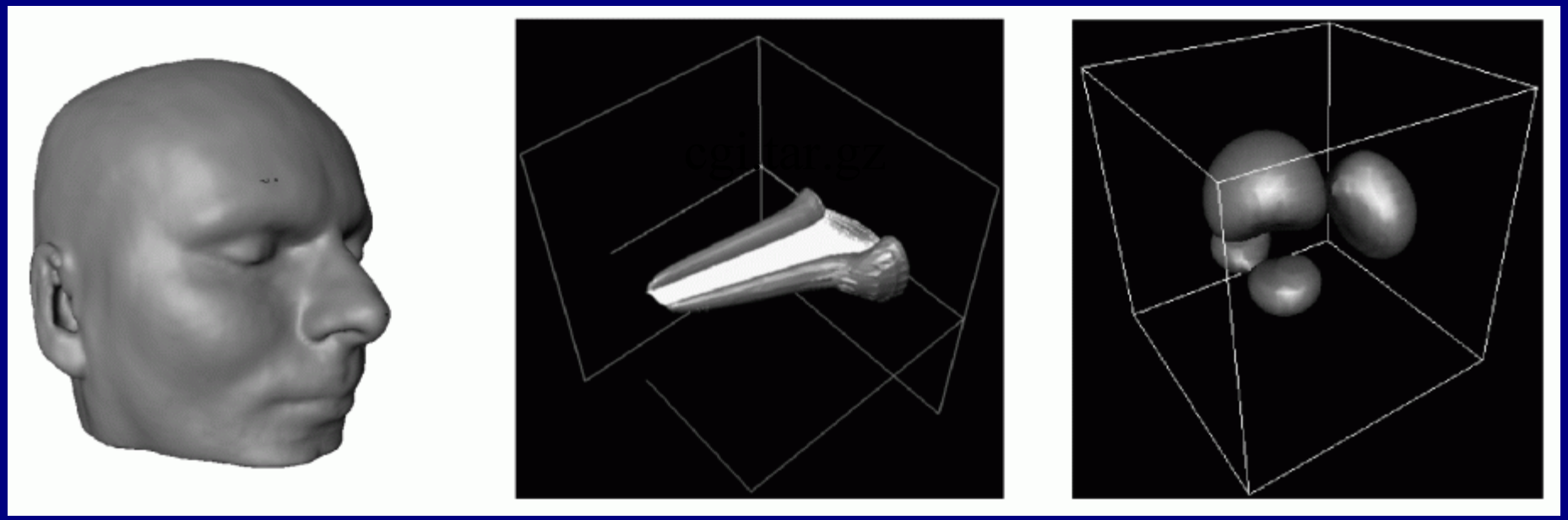
  Talk taken over by Klaus Engel



Progressive Iso-Surfaces for the World Wide Web

Volume visualization: 3D scalar datasets



Medical data
(CT, MRI, PET)

Computational fluid dynamics (CFD)

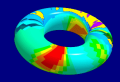
Chemistry
(molecular orbitals)

Isosurfaces: Motivation

Problems for distributed visualization:

- Large size of volume datasets
- Iso-surfaces: large amount of triangles produced by standard algorithms

Visualization Pipeline:



Isosurfaces: Our Solution

Size of datasets:

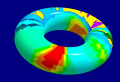
- Store them on a visualization server
- Transfer geometry, not volume data

Number of geometric primitives:

- Multiresolution representation
- Progressive display
- Level of detail (LOD) control

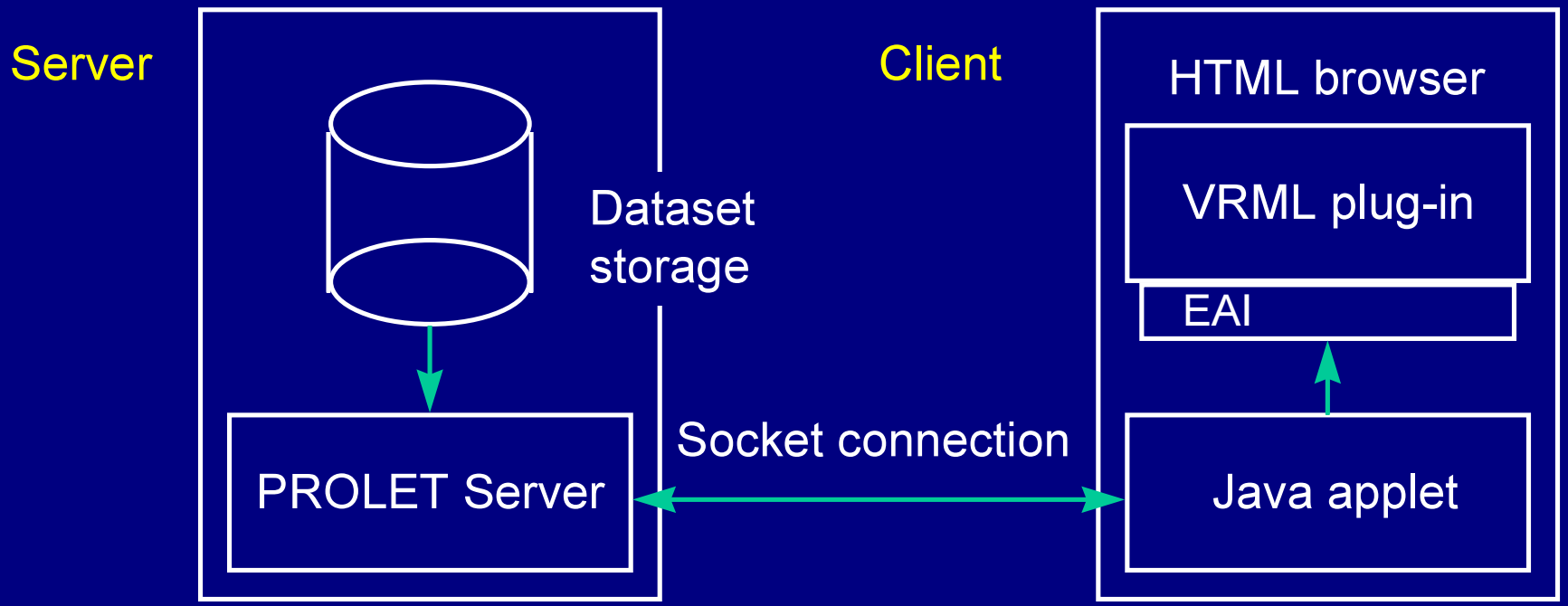
Platform independence:

- Internet standards Java, VRML



PROLET (Progressive Isosurface Applet)

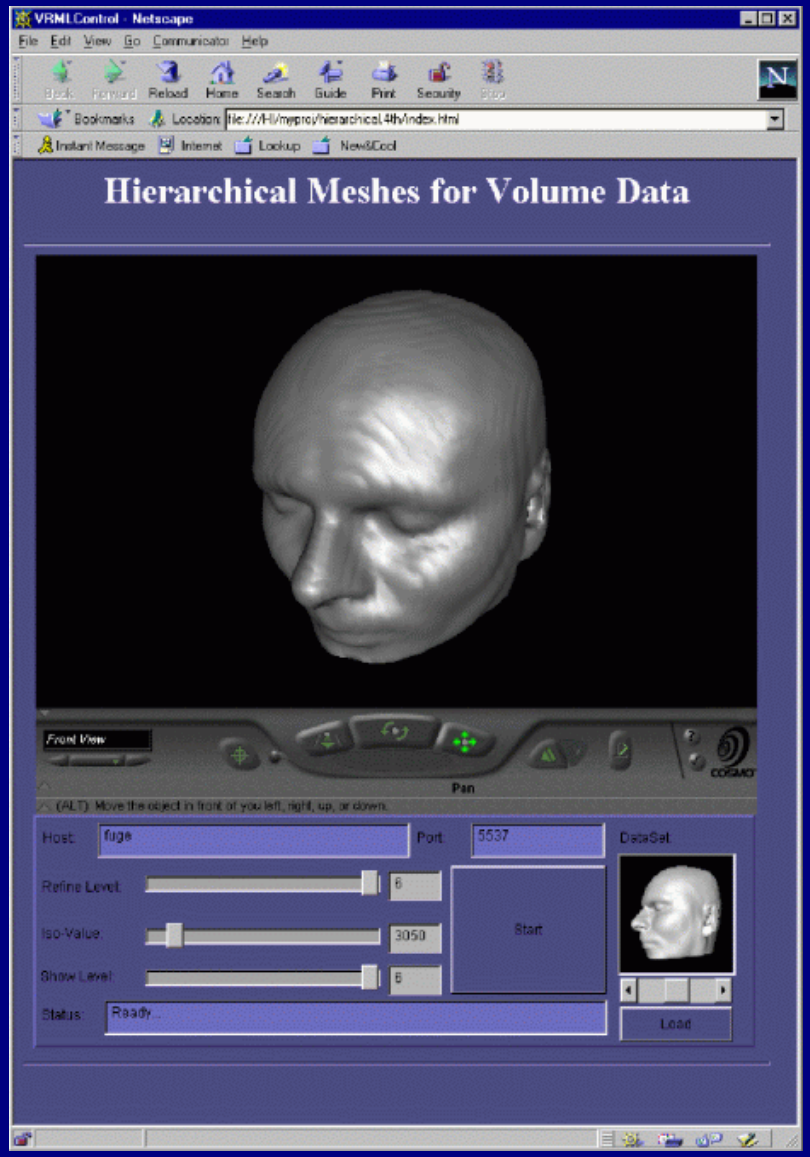
http://www9.informatik.uni-erlangen.de/eng/research/prolet/



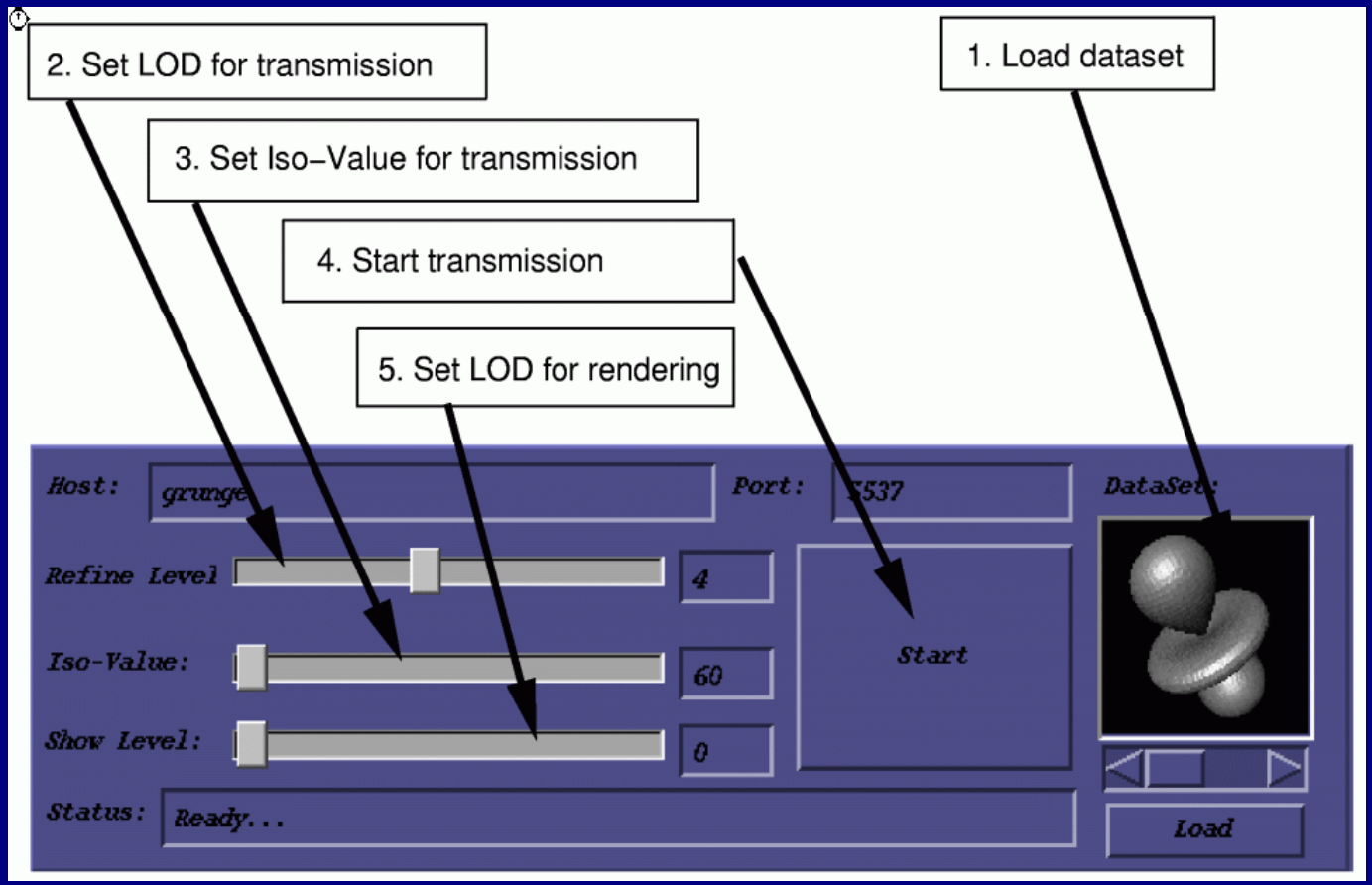
The Prolet Client: General Appearance

VRML plug-in

Java applet

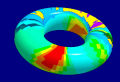


The Prolet Client: User Interface



Building the Scene

- Interface between Java and VRML (External Authoring Interface [EAI])
- VRML scenegraph accessed by Prolet applet through VRML event mechanism
- Prolet applet creates and manipulates geometry dynamically, refining it on demand

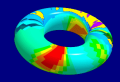


Building the Scene

- Inital approach:

  * build VRML scene as string
  * create scenegraph with *createVrmlFromString* method of *vrml.external.Browser* class
  * send new subgraph to existing VRML group node via *addChildren eventIn* field

- Too slow due to string ops and VRML parsing

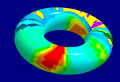


Building the Scene

- Usable approach:

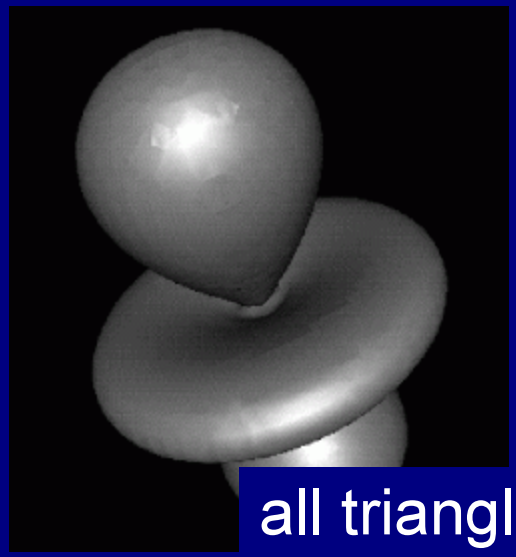
  * provide base VRML scene with empty *IndexedFaceSet* nodes
  * set vertices with *eventIn* field *points* of *IndexedFaceSet* node
  * set indices with *eventIn* field *set_coordIndex* of *IndexedFaceSet* node

- Notably more efficient

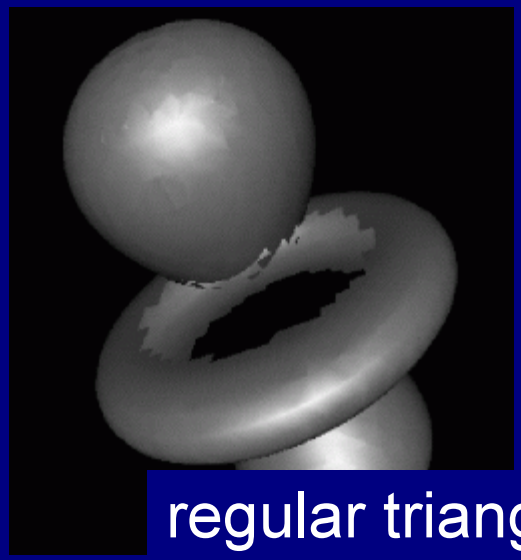


Progressive Refinement

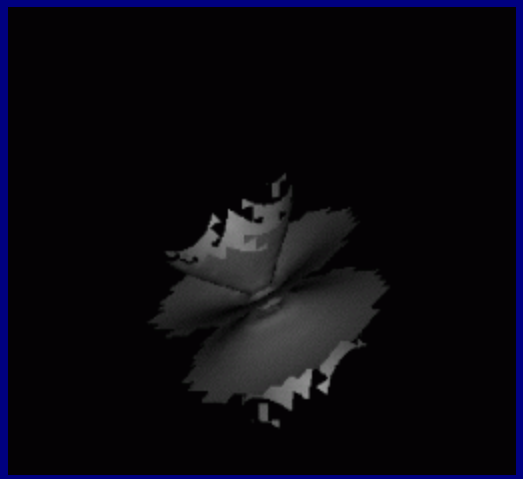
- Transmission of *irregular* and *regular* triangles for each level **m**
- *Irregular* triangles appear only in level **m**
- *Regular* triangles are added to level **m** and all further levels of the isosurface (**m**..**n**)



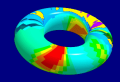
all triangles



regular triangles

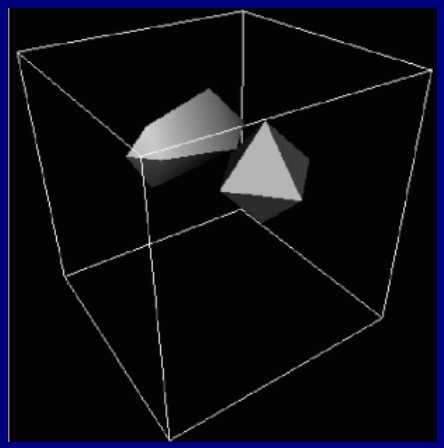


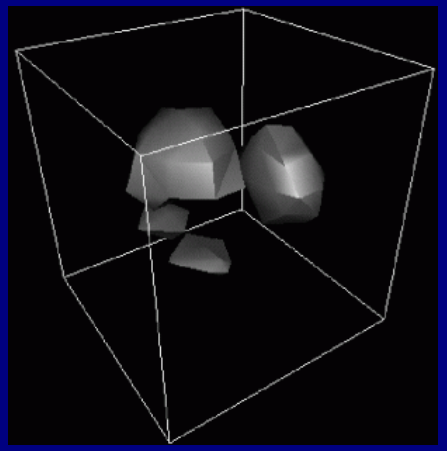
irregular triangles



Isosurface Example: HOMO MO of 1.1-difluoropropene-2

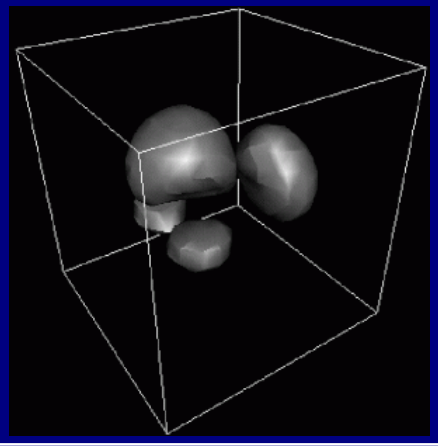
Level 2

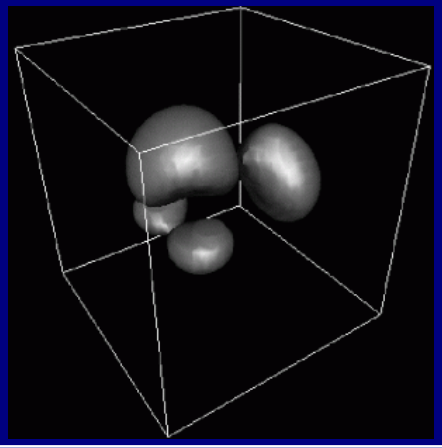




Level 3

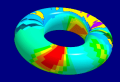
Level 4





Level 5

Iso: 0.01



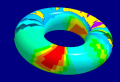
Progressive Isosurface Rendering: Conclusion

Progressive Transmission offers:

- Fast preview of the isosurface
- Additional detail on demand
- Low network load for first impression
- Low overhead

VRML and Java offer:

- Platform independence
- Fast rendering by transparent utilization of 3D-hardware and optimized rendering libraries



Acknowledgments

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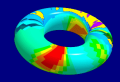
Deutsche Forschungsgemeinschaft DFG

V"D" Digital Library Initiative



More Information

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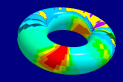
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