CCP4 Molecular Graphics Project
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Aims:

- Molecular structure viewer.
- Electron density viewer.
- Model building/refinement program.
- Picture/movie creator.
General Design:

- High level stuff done in Python.
- Lower level stuff in C/C++
- Python/C++ communication done via SWIG wrappers.
- Uses MMDB (Eugene Krisseneel).
- Uses Clipper (Kevin Cowtan).
- Tcl/Tk GUI.
GUI Considerations:

- GUI with same look and feel as CCP4i.
- Context sensitive menus in graphics window.
Old Prerequisites:

- Tcl/Tk, with BLT and Itcl.
- Python 2.2 or later with working thread support.
- OpenGL (or Mesa).
New Prerequisites:

- OpenGL (or Mesa).
Some basic features:

- View PDB/mmCIF files.

- Download and view PDB/mmCIF over web (and save locally).

- Convert MTZ files to electron density isosurfaces.

- Display all map files supported by CCP4 as electron density isosurfaces.
Model display features:

- Colour by variety of criteria
  - By atom, residue, chain, etc.
  - By atom/residue property.
  - By user defined criteria.

- Draw in various styles, stick, lines, ribbons, etc.
Model display features:

- Define many different atom selections
  - All
  - Chains
  - Residue types
  - Atom types
  - Lots more
Map display features:

- Display electron density as wireframe, cylinders or solid.
- Vary quality of fft calculation on map load.
- Apply symmetry from mtz file to molecule drawing.
- Colour molecules by symmetry transformation.
- Clip to point or atom selection.
- Show unit cell.
Superposition of proteins

- Graph theory structure analysis.

- Whole molecule or selection.

- Two or more molecules.
Some more display features:

- Overlay arbitrary text and images
  - Text with any system font, inc anti-aliased TrueType and PostScript.
  - Text at any size (for scalable and vector fonts).
  - Sub- and super-scripting.
  - Text any colour or combination of colours.
  - Scale/position images.
Images and text
"Vectors":

- Display TLS refinement vectors.
- Display vector between two arbitrary points/atoms.
Nucleic acids display:

- Display nucleic acids just as any other molecule.
- Display as ribbons through phosphate.
- Display as base-pair "blocks".
Surfaces:

- Display molecular surfaces.
- Display electrostatic potential on surface
- (Work by Martin Noble and Jan Gruber).
Output:

- Output screenshots, jpeg, png, tiff, etc.
- Output series of screenshots for making movie.
- Export postscript.
- Export Povray scene description.
Portability:

- Linux: SuSE 8.x, 9.x, Red Hat 7.x, 8.x, 9, Fedora 1,2,3.
- Apple Mac OS X 10.2, 10.3 (10.4?).
- Compaq Tru64 Unix v5.0.
- Irix 6.4.
- Solaris 8.

Current version at http://www.ysbl.york.ac.uk/~ccp4mg/
To Do:

- Incorporate parts of Paul Emsley’s Coot.

- Fix some speed problems, most notably start up time on OS X.

- Fix bugs.
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