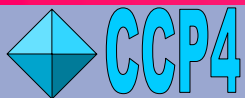


New Developments in the CCP4 Software Suite: v5.0 and beyond



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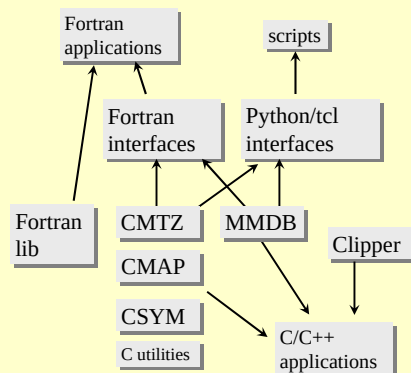


• CCP4 version 5.0

The Collaborative Computational Project No. 4 (CCP4) is one of a number of CCPs based at Daresbury Laboratory, and distributes a software suite for the determination of macromolecular structures by X-ray crystallography. The suite consists of nearly 200 programs, a set of core software libraries and data file formats, plus a graphical user interface **CCP4i**.

CCP4 version 5.0 is a major update of the software suite which is expected to be publicly available in Autumn 2003.

• CCP4 Software library ...



The new CCP4 core libraries are C-based and provide a variety of functions (data handling, access to CCP4 environment and basic crystallographic operations) to C and C++ programs, as well as supporting the existing "legacy" Fortran77 programs.

The new libraries will allow migration to more modern software paradigms (e.g. object-orientation), facilitating the development of new applications whilst also providing the infrastructure for the automation of the structure solution pipeline - both requirements for high-throughput structural genomics projects.

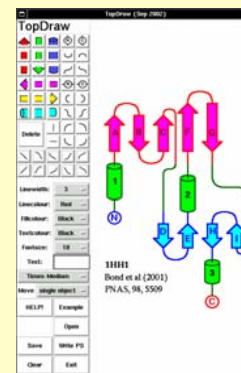
• New and Updated Programs...

New programs include:

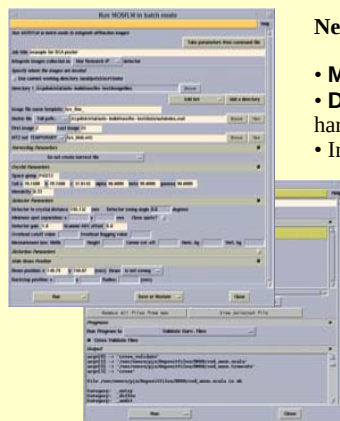
- **topdraw** - sketchpad for drawing protein topology cartoons (Charlie Bond)
- **bulk** - bulk-solvent correction for translation search in AMORE (Andrei Fokine, Guido Capitani, Marcus Grütter, Alexandre Urzhumtsev)
- **dtrek2scala** - convert unmerged D* TREK data to input to scala (Gwyndaf Evans)
- **pdbncur**, **ncont** - utilities to manipulate coordinate files and search for contacts (Eugene Krissinel)
- **cif2xml**, **cross_validate**, **pdb_extract** - utilities for manipulating data harvest files (Pryank Patel and RCSB)

Updated programs include:

- **REFMAC5.2**, **ACORN**, **AMORE**, **MOLREP**, **MOSFLM**, **SCALA**, **OASIS**, **SFCHECK** and many others...



• Updates to CCP4i ...



New interfaces include:

- **Mosflm** - to perform batch mode integration
- **Data Harvesting Manager** - review and manage harvest files
- Interfaces for programs
 - **ArealMol** (solvent accessible areas)
 - **PolarRfn** (rotation function calculation)
 - **ClustalW**

Other changes include:

- Significantly updated Refmac5 interface
- Help text now also displayed as "bubble help"
- New module for Graphics and Viewing Utilities

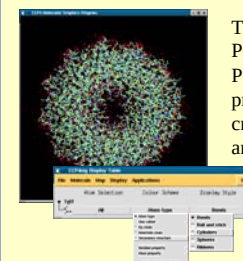
• Supported platforms ...

Supported platforms now include:

- All standard UNIX-, Linux- and Windows-based platforms, plus Mac OS-X
- New in v5.0: support for Linux Intel compilers and Itanium-based systems

• Beyond CCP4 5.0 ...

CCP4mg - Molecular Graphics Project



The CCP4 Molecular Graphics Project "**CCP4mg**" is led by Liz Potterton, with the objective of producing a graphics package that crystallographers can use to solve and analyse their structures

The initial release will focus on display and superposition of structures, with later versions containing tools for model building and refinement.

<http://www.ysbl.york.ac.uk/~lizp/molgraphics.html>

CLIPPER Crystallographic Applications



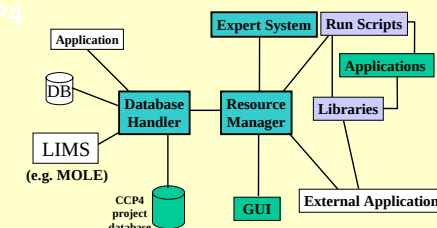
CLIPPER is an independent project led by Kevin Cowtan, to provide a set of object-oriented C++ libraries for crystallographic computation.

Clipper is expected to form the basis of a new generation of advanced applications, such as PIRATE (phase improvement) and BUCCANEER (automatic chain tracing).

Also the CCP4mg project is built using the Clipper libraries

<http://www.ysbl.york.ac.uk/~cowtan/>

Automation and Data Management in CCP4



As part of CCP4's long-term plans to provide an infrastructure for software automation and development of novel applications, migration towards a modular system is envisaged. This "open architecture" will provide modules for database access as well as "toolboxes" of basic crystallographic functions.

The CCP4 project is supported by the BBSRC, by income from commercial distribution of the software and by CCLRC Daresbury Laboratory. CCP4 would also like to thank the many people who have contributed to the project since its inception. For more information about CCP4, please visit our web pages at <http://www.ccp4.ac.uk>