



CCP4 Release 5.0

Peter Briggs

CCP4/CCLRC Daresbury Laboratory

New Core Software Libraries

Core libraries provide common functions to the programs:

- CCP4 environment (e.g. keyworded input)
- Read/write standard file formats (e.g. MTZ, PDB, maps)
- Basic crystallographic functions (e.g. symmetry info)

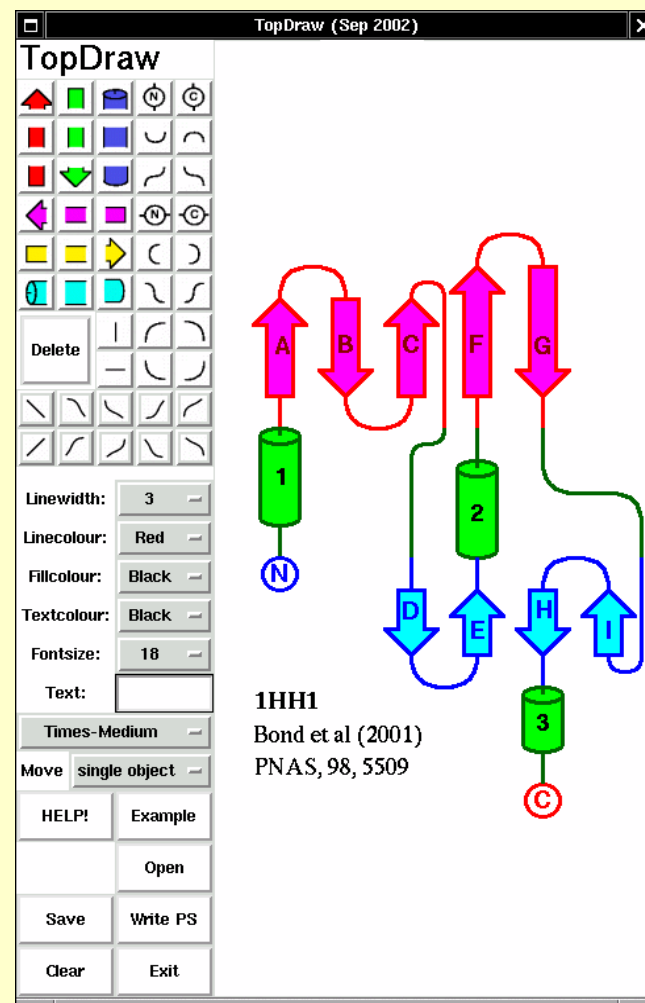
New CCP4 libraries:

- Support the existing Fortran77 “legacy” programs
- Make functions available to different programming languages
- Provide basis for improved software infrastructure in future

Useful for software developers, of little interest to general users!

New Programs

- **topdraw** - sketchpad for drawing protein topology cartoons (*Charlie Bond*)
- **dtrek2scala** - convert unmerged D*TREK data to input into scala (*Gwyndaf Evans*)
- **bulk** - bulk-solvent correction for translation search in AMoRe (*Andrei Fokine, Cuido Capitani, Marcus Grütter, Alexandre Urzhumtsev*)
- **ncont** - search for protein contacts
- **pdbcur** - manipulate PDB files (*Eugene Krissinel*)



Updated Programs and Other Changes

Updated programs include:

- **REFMAC5 . 2** (plus major updates to the monomer library)
- **ACORN, AMORE, MOLREP, SCALA, OASIS, SFCHECK ...**
- many other minor updates

New supported platforms:

- Intel compilers on Linux
- Itanium systems (SGI, Hewlett-Packard)

Updated documentation:

- New CCP4i-based tutorials (*Maria Turkenburg, Eleanor Dodson*)
- “Maths for crystallographers”

Updates to CCP4i

New interfaces:

- **Mosflm** - batch mode integration
- **ArealMol** - solvent accessible area calculation
- **PolarRFn** - rotation function calculation
- **ClustalW** * - sequence alignments

Other changes:

- Significantly updated **Refmac** interface
- Help text also displayed as “balloon help”
- New module **Graphics and Viewing Utilities**
- *plus many other more minor updates and bugfixes*

* *ClustalW* program not distributed as part of CCP4.

Run MOSFLM in batch mode

Run MOSFLM in batch mode to integrate diffraction images

Take parameters from command file

Job title: example for BCA poster

Integrate images collected on: Mar Research IP

Specify where the images are located

Use current working directory /amd/pxfs5/scr1/mdw

Directory 1: /ccpdisk/xtal/auto-build/mosflm-test/imagefiles

Image file name template: lys_fine

Matrix file: Full path... /ccpdisk/xtal/auto-build/mosflm-test/data/autoindex.mat

First image: 2 Last image: 51

MTZ out: TEMPORARY

Harvesting Parameters

Do not create harvest file

Crystal Parameters

Space group: P43212

Cell a: 78.1508 b: 78.1508 c: 37.0143 alpha: 90.0000 beta: 90.0000 gamma: 90.0000

Mosaicity: 0.33

Detector Parameters

Detector to crystal distance: 195.132 mm Detector swing angle: 0.0 degrees

Minimum spot separation: x y Close spots?

Detector gain: 1.8 Scanner ADC offset: 5.0

Overload cutoff value Overload flagging value

Measurement box: Width Height Corner cut-off Horiz. bg Vert. bg

Distortion Parameters

Main Beam Position

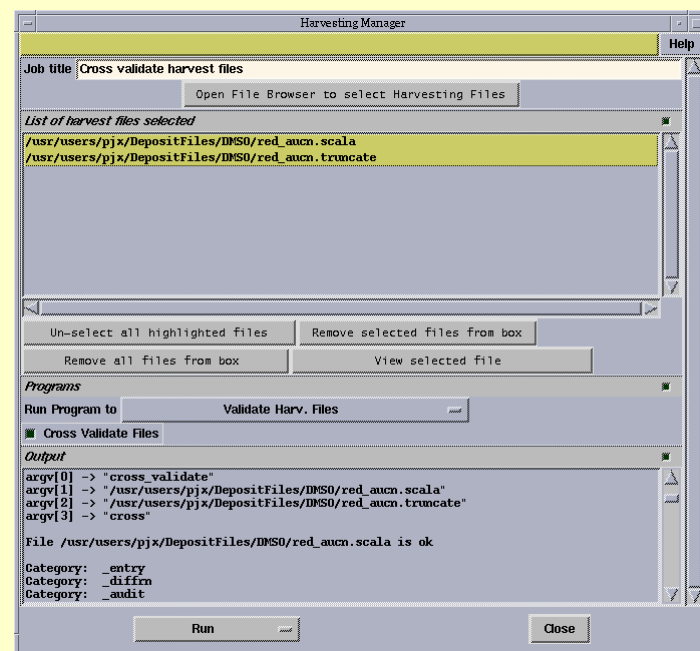
Beam position: x: 149.79 y: 150.87 (mm) Beam: is not swung

Backstop position: x y Radius: (mm)

Run Save or Restore Close

Updates to Data Harvesting (Pryank Patel)

- Data Harvesting now enabled under Windows
- New harvesting based applications include:
 - **cif2xml** - convert CCIF harvest files into XML format
 - **cross_validate** - check harvest files for consistency
 - **PDB_EXTRACT** - generate harvesting information from CCP4 logfiles (RCSB)
- **Data Harvesting Management Tool**
 - CCP4i-based
 - manage/review harvesting files
 - interface to **pdb_extract**, **cif2xml**, **cross_validate**



CCP4 5.0 - when will it be available?

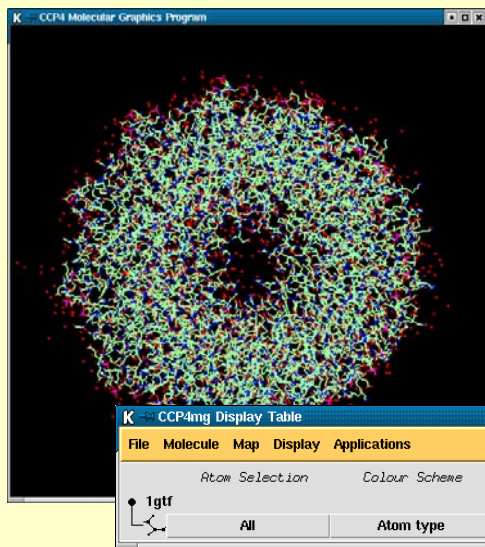
- **Target release date end of September 2003**
- **Watch for announcements on “ccp4bb”**

For more information: come and see our poster (#8)

or

Talk to us at the CCP4 stand in the marquee

Developments within the CCP4 software suite beyond 5.0



CCP4 Molecular Graphics CCP4mg

- aims to produce graphics package for solution and analysis of macromolecular structures
- <http://www.yesbl.york.ac.uk/~lizp/molgraphics.html>

CLIPPER-based Crystallographic Applications

- *Clipper* = Kevin Cowtan's advanced software libraries for crystallographic computation
- Forthcoming applications PIRATE (phase improvement) and BUCCANEER (automatic chain tracing)
- <http://www.yesbl.york.ac.uk/~cowtan>



CCP4 Version 5.0: Acknowledgements

- Everyone who has contributed new and updated software, bug fixes and enhancements... far too many to list here!

- **Testers (in no particular order!):**

Clemens Vornrhein (Global Phasing)

Ian Tickle, Andrew Sharf (Astex)

Phil Evans (MRC-LMB)

Eleanor Dodson, Maria Turkenburg, Liz Potterton (York University)

Martin Noble (Oxford University)

Huangwang Yang (RCSB)

Jawahar Swaminathan (EBI)

Ezra Peisach (Brandeis University)

- Pryank Patel
- CCP4 DL staff
- *CCP4 is supported by BBSRC, income from commercial distribution of the software and by CCLRC Daresbury Laboratory*