CCP4 Release 5.0

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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!

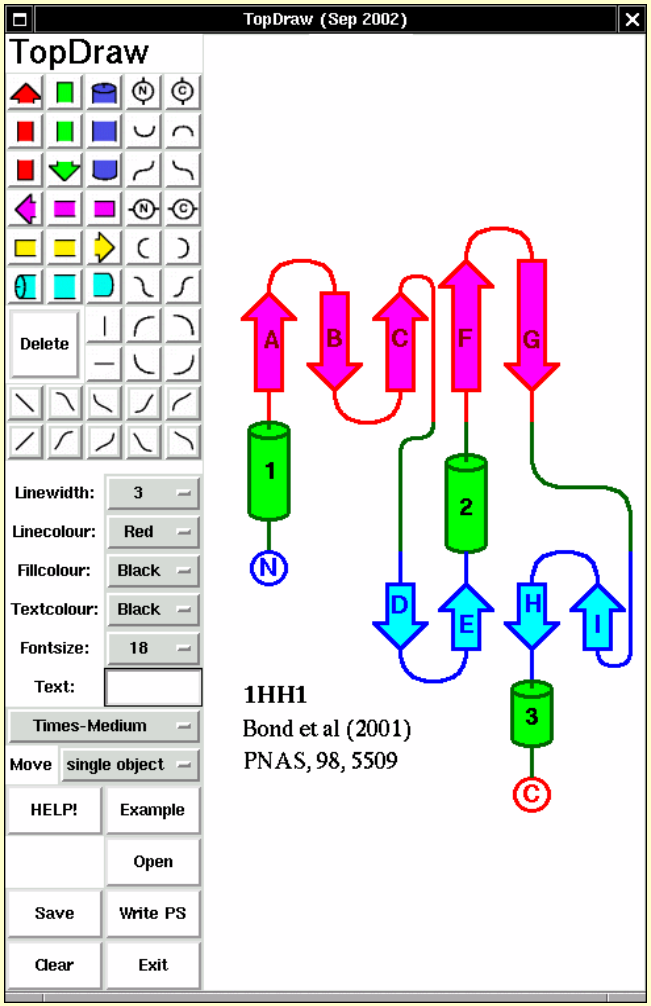
New Programs

- **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, Alexendre 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)

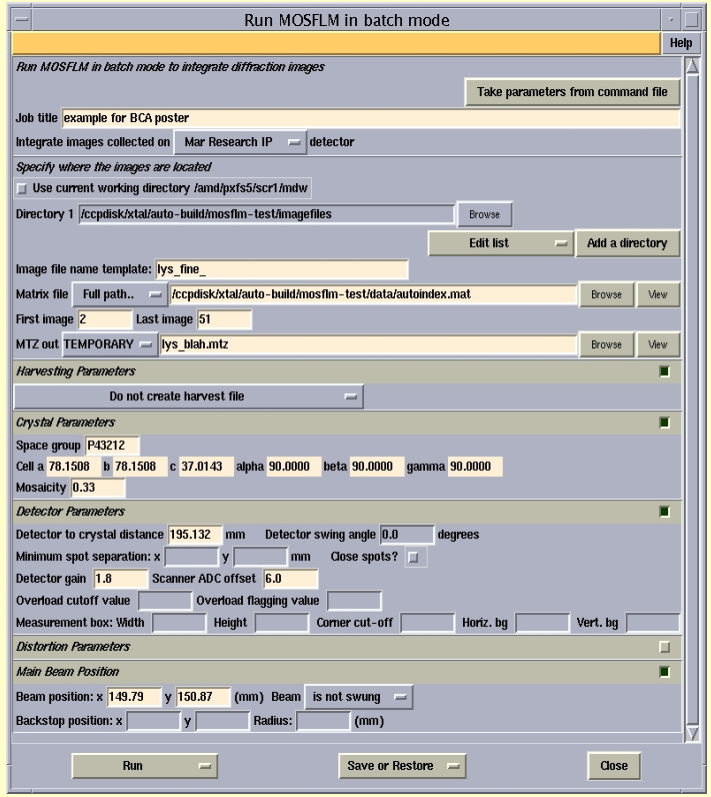
Updated documentation:

- 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***

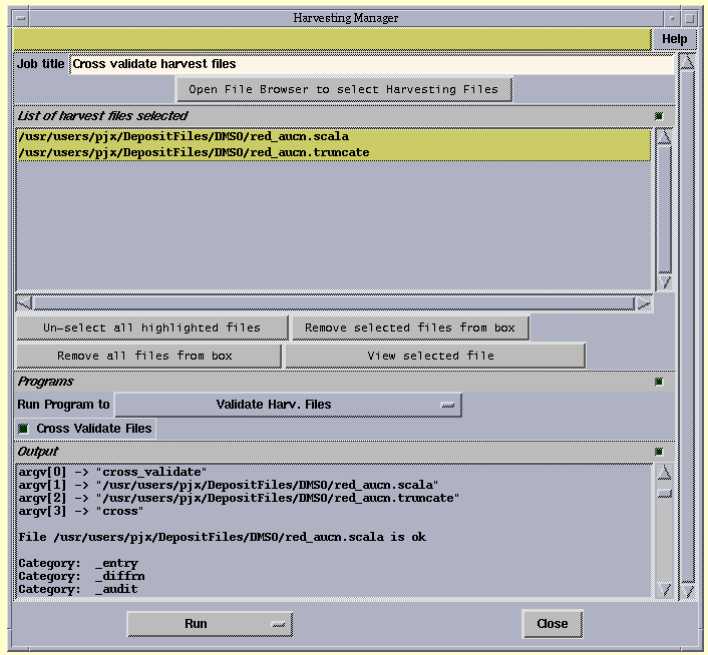
** ClustalW program <u>not</u> distrbuted as part of CCP4.*

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?

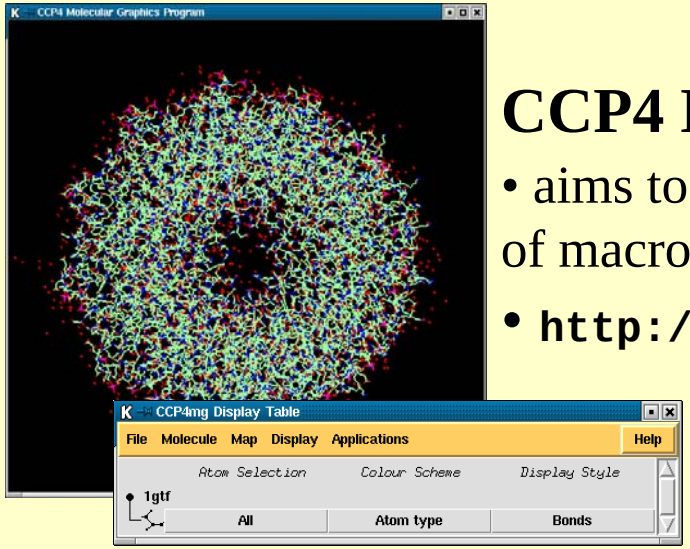
- **Target release date end of September 2003**
- **Watch for announcements on "ccp4bb"**

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.ysbl.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.ysbl.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!):**
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Ezra Peisach (Brandeis University)

• Pryank Patel
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