News of CCP4 Release 6.1

Peter Briggs, Martyn Winn, Charles Ballard, Francois Remacle, Norman Stein and Ronan Keegan

CCP4, CSE Department, STFC Daresbury Laboratory, Warrington WA4 4AD
Email: ccp4@dl.ac.uk

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1 Introduction

The current release of the CCP4 software suite is version 6.0.2, which was made available in December 2006 and which has previously been described in some detail in an article in newsletter 44. This article outlines the new and updated programs and features that are currently scheduled for inclusion in the next major release of CCP4, version 6.1, due out later in 2008.

2 Major Changes in CCP4 6.1

2.1 New programs

A number of significant new programs will be included in CCP4 6.1:

- **AFRO**: a program for calculating E_A values (the normalised heavy atom contribution) from SAD, MAD and SIRAS data.
- **BUCCANEER**: statistical model building program that can be used to trace protein structures in electron density maps by identifying connected alpha-carbon positions using a likelihood-based density target.
- **CTRUNCATE**: a program for converting intensities to structure factors and checking data quality. CTRUNCATE is intended to supersede the existing TRUNCATE program.
- **CRUNCH2**: program for determining the substructure of the anomalous scatterers or heavy atoms.
- **MrBUMP**: an automated pipeline for molecular replacement developed by Ronan Keegan and Martyn Winn, which includes search model retrieval and search model preparation.
- **PISA**: a standalone version of Eugene Krissinel's PISA (Protein Interfaces, Surfaces and Assemblies) program that is a useful for examining various characteristics of protein packing and other interactions. Previously the PISA functionality was only available as a web-based service from the EBI.
- **POINTLESS**: program for Laue and Patterson group determination from unmerged reflection data, as well as a number of subsidary functions including: reflection format conversion, checking and reindexing of reflection data against a reference set, and apply a pre-selected reindexing matrix.
- **RAPPER**: program for generating protein conformers by discrete sampling of likely conformers within a given set of restraints. It can be applied to a number of problems, for example: *ab initio* loop building, comparative modelling and C• -trace modelling. It can also be used to build and refine conformers using X-ray crystallographic data.

The RAMPAGE module of RAPPER also provides an analysis tool that generates Ramchrandran plots which are more consistent with current models than those in PROCHECK.

- **SEQUINS**: SEQUence INSertion detection program that performs sequence validation by comparing model side chains against electron density. It can be used after molecular replacement or to validate structures in the PDB.
- **XIA2**: an expert system for performing automated reduction and analysis of X-ray diffraction image data with minimal user input. It is aimed at two principal sets of users: novice users with little knowledge or experience of data processing, and expert users who wish to process higher volumes of data.

There are also new utility programs scheduled for inclusion:

- **IDIFFDISP**: a standalone viewer for raw diffraction images which is intended as a replacement for the old IPDISP program.
- **MTZ2CIF**: a utility that generates mmCIF reflection files suitable for deposition, and is intended to replace OUTPUT CIF option of MTZ2VARIOUS.
- **R500**: utility for correcting REMARK 500 lines in PDB files before submission to a deposition site.
- **SEQWT**: a program that estimates protein molecular weight from the sequence
- **SYMCONV**: a utility for interrogating the CCP4 symmetry libraries in order to look up information about spacegroups and symmetry operations in various formats.
- **BAUBLES**: a utility for re-rendering CCP4 log files into HTML markup. Baubles will be integrated into CCP4i.

It should be noted that many of these programs have been available for some time already, either via the CCP4 Prerelease Pages at http://www.ccp4.ac.uk/prerelease/ or via their own project-specific pages. However, their inclusion in CCP4 6.1 means that users will no longer have to download and install them separately.

2.2 Updated Programs

In addition to the new programs outlined in the previous section there are various updates to many of the existing programs in the suite. These include:

- **PHASER** 2.1.2 (this version covers MR, SAD and combined MR and SAD)
- **REFMAC** 5.4.0067
- **SCALA** 3.3.1
- **SFCHECK** 7.02.6
- **MOLREP** 10.1.7
- **MOSFLM** 7.0.2 (along with the new iMOSFLM interface)
- **OASIS** updated to OASIS-2006
- **PDB_EXTRACT** 3.0
- **CRANK** 1.20

Please note that these version numbers are correct at the time of writing but may be superseded by newer versions before CCP4 6.1 is finally released. The latest versions of COOT and CCP4MG will also be made available for download with CCP4 6.1.

2.3 Changes to Graphical User Interface CCP4i

The improvements and changes to CCP4i are described extensively elsewhere in this newsletter. They include new task interfaces for the new programs plus many new core features and enhancements.

2.4 New Libraries

The release of CCP4 6.1 will include the new **DiffractionImage** library, which provides a set of C++ functions (plus wrappers in different languages including Tcl and Python) for handling diffraction image data from a variety of sources.

DiffractionImage also comes with a set of utility programs:

- **diffdump**: displays all the "standard" information from a specific diffraction image file
- **printpeaks**: prints a list of peaks found on an image
- **automask**: automatically generate a backstop mask from a an image
- **diff2jpeg**: generate a JPEG from an image file

2.5 Deprecated and Withdrawn Programs

As part of the CCP4 6.1 release a number of programs have been designated as "deprecated", in anticipation of removing them completely from future releases. These programs have either been superseded by superior programs, or have fallen out of mainstream use. They are:

- BEAST (replaced by Phaser)
- ROTAPREP (replaced by Combat)
- ARP_WATERS (the latest version of ARP/wARP should be used instead)
- XLOGGRAPH (replaced by loggraph)
- IPDISP (replaced by idiffdisp)
- BPLOT, POLYPOSE, RSEARCH, RESTRAIN, XDLMAPMAN and XDLDATAMAN

The source code of deprecated programs will still be included for download, however they will not be built as part of the standard installation process and will not be included in the binary distributions that CCP4 provides.

2.6 Other changes and new features

There are various miscellaneous changes and features scheduled for CCP4 6.1:

- **Dependency on Fortran 90**
  The latest versions of REFMAC (5.3+) and MOLREP (10+) now require a Fortran 90 compiler in order to build. This should only affect users who build the suite from source code.
  The CCP4 configure will check for Fortran 90 support and will automatically disable the REFMAC and MOLREP builds if it is not available.

- **Update Alert Mechanism**
  It is intended to implement an "update alert mechanism" as part of CCP4 6.1, which will automatically notify users when bug fixes or updated program versions become

available on the CCP4 server. Although the details are still being worked out, the intention is to help users keep their CCP4 distributions more up-to-date in between major releases of the suite.

- **InstallShield installation wizard for Linux systems**
  For CCP4 6.1 an InstallShield-based installer (similar to that already used for Microsoft Windows platforms) will be available for installing pre-compiled executables onto Linux systems.

3 Current Status and Availability

At the time of writing (January 2008) there are currently still a few components and features which have not yet been fully integrated into the suite, however initial test versions have been made and are undergoing testing with a selected group of developers and users.

It is planned that a small number of additional test releases will be made over the next couple of months ahead of the full public release. If you are interested in trying out a trial version of 6.1 then please contact ccp4@dl.ac.uk.

CCP4 6.1 is scheduled for a full public release sometime in spring 2008. Watch for announcements on the CCP4bb mailing list and other crystallographic lists, or check the CCP4 home page for news.

Finally, this article reflects our current state of knowledge about the expected content of CCP4 6.1, however it is possible that there may be some changes before the public release. It is recommended therefore that you check the list of significant changes that is distributed with the suite and linked from the main documentation index.

4 Acknowledgements

The CCP4 project is a collaborative effort and continues to thrive through generous contributions of time, energy and software from members of the UK and international PX communities. Unfortunately time and space do not permit the acknowledgement here of all these valuable contributions, however a list of acknowledgements is included in the current release, and acknowledgements for the specific developments described in this article are given below:

- AFRO is developed by Navraj Pannu; CRUNCH2 is developed by Jan Pieter Abrahams (Leiden University)
- BUCCANEER and SEQUINS are developed by Kevin Cowtan (University of York)
- CTRUNCATE is developed by Norman Stein (CCP4, Daresbury Laboratory)
- MrBump is developed by Ronan Keegan and Martyn Winn (CCP4, Daresbury Laboratory)
- PISA is developed by Eugene Krissinel (MSD-EBI)
- SCALA and POINTLESS are developed by Phil Evans (MRC-LMB Cambridge).
- RAPPER is developed by Nicholas Furnham, Paul de Bakker, Mark DePristo, Reshma Shetty, Swanand Gore and Tom Blundell (University of Cambridge)
- XIA2 is developed by Graeme Winter (CSE, Daresbury Laboratory)

- IDIFFDISP is developed by Francois Remacle (CCP4, Daresbury Laboratory). The DiffractionImage library is developed by Francois Remacle in collaboration with Graeme Winter.
- MTZ2CIF and SYMCONV are developed by Peter Briggs. BAUBLES has been developed by Peter Briggs in collaboration with Kevin Cowtan and Phil Evans.
- R500 is developed by Kim Henrick (MSD-EBI)
- SEQWT is developed by Eleanor Dodson (University of York)
- PHASER is developed by Randy Read's group (Wellcome Trust, Cambridge).
- REFMAC5 is developed by Garib Murshudov's group (University of York)
- SFCHECK and MOLREP are developed by Alexei Vagin (University of York)
- OASIS is developed by Tao Zhang *et al* (Beijing National Laboratory for Condensed Matter Physics) and Quan Hao (Cornell University)
- PDB_EXTRACT is developed by Huanwang Yang (RCSB PDB)
- CRANK is developed by Navraj Pannu (Leiden University)
- CCP4mg is developed by Liz Potterton and Stuart McNicholas (York University)
- COOT is developed by Paul Emsley (Oxford University)
- MOSFLM is developed by Harry Powell and Andrew Leslie; iMOSFLM is currently developed by Luke Kontogiannis (MRC-LMB Cambridge)
- CCP4i is maintained and developed by the CCP4 group at Daresbury

The CCP4 suite is maintained, developed and released by the CCP4 group in the Computational Science and Engineering Department (CSED) at STFC Daresbury Laboratory, and comprises Charles Ballard, Peter Briggs, Maeri Howard, Ronan Keegan, Francois Remacle, Norman Stein and Martyn Winn.

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