New Developments in the CCP4 Graphical User Interface

Peter J. Briggs, Liz Potterton[*], Pryank Patel, Alun Ashton, Charles Ballard, Martyn Winn

CLRC Daresbury Laboratory, Warrington, Cheshire WA4 4AD, UK
[*] **Structural Biology Laboratory, Department of Chemistry, University of York, YO10 5YW.**

• Automating Tasks ...

Automation efforts within CCP4i have so far taken two particular approaches - the first is to add automatic functionality within existing tasks, the second to facilitate the automatic transfer of information between separate tasks. An example of each are outlined below.

Example 1: Automatic data passing via XML

When using the **MOLREP** (*A. Vagin, A. Teplyakov, J. Appl. Cryst. (1997) 30 pp1022-1025*) to find Molecular Replacement (MR) solutions, it helps to know details such as the number of monomers expected in the asymmetric unit, and any pseudo-translation vectors.

This information can be found by first running two other tasks (**Matthews_Coeff** and **MRAnalyse**), and the relevant data from these are now written automatically to XML files.

XML (eXtensible Markup Language) is a way of marking up data in an extensible and portable format, and a number of standard tools exist for reading and manipulating it. Using these tools, the MOLREP task will now read the data directly, avoiding the need for manual transfer of the information from the logfiles (and any associated transcription errors).

Example 2: CAD AutoReindexing

When merging many datasets into a single MTZ file using the **CAD** task, it is occasionally possible that the reflections in one of the datasets may have been indexed differently to those in the others.
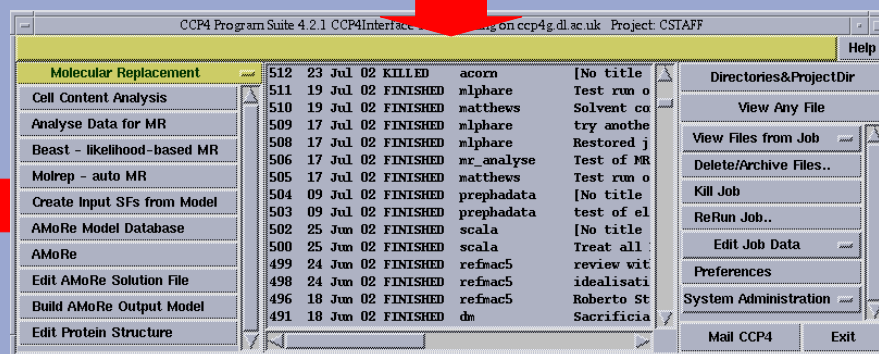
The CAD task can now automatically check the consistency of the indexing schemes, and if necessary correctly reindex them. Detecting and correcting this error can prevent serious problems later, saving valuable time for the user.

• New Tasks ...

Amongst others, new tasks in the latest version of CCP4i include **GetProt** (now SAPHIRE), which allows downloading and editing of protein sequence information, and an interface to the **AstexViewer**, a Java application for displaying maps and protein-ligand complexes.

• Introduction to CCP4i

The Collaborative Computational Project No. 4 (CCP4) is one of a number of CCPs based at Daresbury Laboratory, and distributes a suite of over 150 programs for the determination of macromolecular structures by X-ray crystallography.
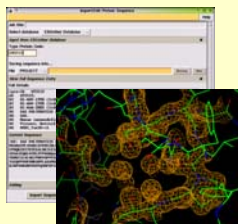
Since 1999 CCP4 has also distributed a graphical user interface called **CCP4i**, which was originally developed by Liz Potterton at the University of York. **CCP4i** sits on top of the programs and facilitates the use of the software by presenting clear interfaces for each crystallographic task. Its ease of use, as well as a number of useful additional features (in particular the project history database) have won it many converts amongst both novice and expert users.

Since March 2000 maintenance and development of **CCP4i** has passed to the CCP4 staff based at Daresbury Laboratory, with Peter Briggs as chief developer. This poster outlines some of the major developments within **CCP4i** in the current release of the CCP4 software suite (version 4.2, released in April 2002), as well as some of the projects planned for the next release.

• CCP4 Database ...

The Project History Database (PHdb) within CCP4i is one of its most useful utilities, keeping track of the results from all the jobs within each structure determination project.

In the next release of CCP4i the database manager will be split off from the main CCP4i process, allowing extensions in future to distributed computing environments such as The Grid, and enabling interactions with other databases (such as mySQL) and other external applications (for example the data processing package MOSFLM).
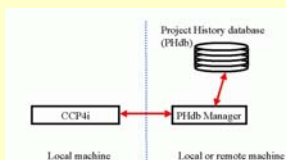
• Utilities ...

MapSlicer

MapSlicer is an interactive viewer for contoured 2-D sections through CCP4-format map files. It allows the display of single sections or "slabs" of multiple superimposed sections, and can easily swap between x, y and z axes. When viewing Patterson maps, it can also jump quickly to the appropriate Harker sections.
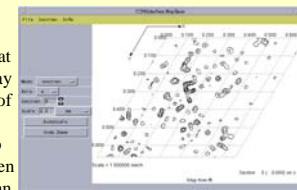
Task Installer

A number of external software projects are now providing CCP4i task interfaces for their own programs, for example the automated model-building package **ARP/wARP** (see *http://www.arp-warp.org*).
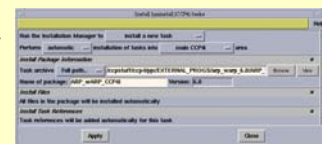
The Task Installer utility makes it easy for developers to export these "3rd party" interfaces. Various features such as version tracking and file backup ensure that the tasks are properly installed and that the user can easily update or remove the relevant files.

MTZ Hierarchical Viewer

MTZ files store columns of reflection data derived from X-ray diffraction images collected during experiments (*e.g.* structure factor amplitudes) and from the subsequent structure determination process (*e.g.* phases).

Organising this data is increasingly important, and to this end the new libraries being developed by CCP4 to handle it will impose a hierarchy of associations. The viewer will present this hierarchy as a tree, making it easier for the user to visualise the data - as well as functioning as a selection tool and as an editor.