Agenda

Meeting title:	CCP4 Working Group 2 meeting
Date:	Wednesday 8th July 2015 **Time:** 11:00 – 16.00
Location:	LMB Cambridge, Francis Crick Avenue, Cambridge Biomedical Campus
Circulation:	ccp4wg2@stfc.ac.uk
Present:	Jon Agirre (JA), Charles Ballard (CB), Arnaud Basle (AB), Ben Bax (BB), David Brown (DB), David Damerell (DD), Judit Debreczeni (JD), Eleanor Dodson (EJD), Paul Emsley (PEM), Phil Evans (PRE), Eugene Krissinel (EK), Andrey Lebedev (ALB), Ed Lowe (EL), Airlie McCoy (AMC), Karen McIntyre (KM), Rob Nicholls (RN), Stuart McNicholas (SMN), Andrew Purkiss (AP), Christopher Roth (CR), Paul Rowland (PR), Ivo Tews (ITE), Ville Uski (VU), Melanie Vollmar (MV), Pamela Williams (PW), Marcin Wodjyr (DLS)
Apologies:	Svetlana Antonyuk, Gwyndaf Evans, Vilmos Fulop, Mike Hough, Johan Turkenburg, Keith Wilson

WG2 meeting

1. Approval of minutes from the Cambridge WG2 meeting 28/1/15
2. Chairs report (Ivo Tews)
3. What's New in CCP4 Core Group, CCP4 6.5 download, Schools, Web pages (Eugene Krissinel)
4. CCP4 Online (Ville Uski)
5. Acta Cryst Special Issue Phasing (Airlie McCoy, Charles Ballard)
6. SW2016 on **Protein-Ligand Complexes: Understanding Biological Chemistry** (Judith Debreczeni, Paul Emsley)
7. AOB
8. Take note of the date of the next meeting (proposal 30.9.2015)

WG2/Gui2 meeting

9. CCP4 Overview (Dave Brown)
10. CCP4 Core group activities on Gui2, implementation, rollout (Andrey Lebedev)
11. CCP4 Gui2 present capabilities (Jon Agirre)

Minutes

1. **Approval of minutes from the Cambridge WG2 meeting 28/1/15**

The minutes from the Cambridge WG2 meeting 28/1/15 were approved.

2. **Chairs report (Ivo Tews)**

Participation and representation of WG2 at the Cosneners Developers meeting. The meeting was focussed on three main topics: ligands, Dials, and GUI2. Also presence at the accompanying Exec meeting at Coseners. The position for WG2 is to promote, alpha test, and comment on software, aside of the classic functions of organising the Study weekend and commenting on workshops and publicity etc.

From the developers meeting: DIALS is now used in XIA2 and running stable, the attention for WG2 now should focus on ways to promote DIALS and spread its use; the proposal to feature this at the next WG2 meeting was agreed. Specific feedback was given on the Gui2 developments from a WG2 viewpoint, mostly concerning intuitively of the display, tooltips and help functionality.

Further presence at the Diamond MX user group meeting and presentation at the South Western Structural Biology Conference in Brighton (SWSBC), At the latter, an outline on membership and roles of working groups was given as WG1 being PIs, with a meeting along the annual study weekend, and WG2 looking to recruit / extend membership from active users of the software.

The proposal was made to extend the function of the mailing list from use to call WG2 meetings to serve the secondary function to inform users on new developments and thus provide a link to the active community. This proposal was met with agreement. Two steps will be taken:

1. Sign up representatives from the Diamond BAGS and other large groups so that information gets disseminated
2. Mail to subscribers who have not attended a WG2 meeting in previous years to confirm if they wish to receive information on WG2 activities, as a secondary function of this mailing list (otherwise remove)

Report on status of CCP4 webpages, feeding back some comments from Dave Waterman. The Web pages have no CMS and are edited directly at present (although some pages are automatically updated). There is some contents broken, and several pages are rough around the edges or out-dated, developers are are a bit of a dumping ground, and it is manual job to fix all this individually. To request updates, one must feedback inaccurate information to the core team at ccp4@ccp4.ac.uk.

A new development should include a CMS, allow developers to provide documentation, and provide developers areas, and appropriate feedback mechanisms. An overhaul is a large job but urgently needs doing (already met with agreement in Exec). Responsibility lies with Eugene.

3. **What's New in CCP4 Core Group, Meetings and Summer Schools (Eugene Krissinel)**

Since launch of CCP4-6.5 (18.12.2014), 13 updates and an off-line updater were released. The CCP4-6.5 windows 32-bit version was released 23 June 2015.

Review of the stats for download show that the average user does not update after installation. Proposal is to use pop-up messages to insure users have an up-to-date installation (and also avoids reporting of errors that are already fixed).

CCP4 and i2 have common updates since early 6.5; PRE: update policy may need updating in GUI2.

CCP4 7.0 is in preparation, and is planned to include integration of GUI2, DIALS, Shelx as well as Archimboldo_lite and PDB_REDO, plus many other updates.

CCP4 website was approved for overhaul, and the update was specified with an external designer. Now looking for a designer to provide framework, CMS and implement. This should be done concurrent with release of 7.0.

Workshops are popular, well attended and over-subscribed. Because their number increases, one would require further volunteers / support. Further, the up-coming release of GUI2 will require road shows. Workshops organized or planned were CeBEM in Uruguay (6-16 April), APS in Argonne (16-23 June), NJUST in Nanjing (12-20 Sept), OIST in Okinawa (2-8 Nov), DIAMOND (Dec); Invited courses were / are Oulu (May), Madrid (May), Biostruct-X in Hungary (Dec). CCP4 was represented in the BCA, SWSBG, ACA and ECM conferences with talks, stands or posters.

Kyle Stevenson will join CCP4 core starting 3 August (windows background).

4. CCP4 Online Web Services (Ville Uski, Eugene Krissinel)

Web services are required to provide access to large, up-to-date databases, and latest software; they are an addition to the diverse CCP4 portfolio. The utilisation of CCP4 Webservices remains high, with Linux cluster of 160 cores and SGE queuing system; 128 cores have been newly acquired. CCP4 also explore SCD resources (SCARF) for more power, but this requires solving some technical details.

Currently CCP4 provide four web-services: Balbes and MrBUMP for molecular replacement, Zanuda for space group validation, and jsPISA for quaternary structure identification. Usage statistics show that Bables is the most popular service, with about 100 users per month. New jsrview output was demonstrated. The new SHELX interface uses javascript to read reflection files.

Webservices will very soon provide for SHELX & AMPLE (both under testing), as well as CRANK2. Later in the year, services will provide LRSR, a low-resolution refinement pipeline (Oleg Kovalevsky), and a programmable RESTful web API. Access to web-services at http://www.ccp4.ac.uk/ccp4online.

5. CCP4 SW 2015 “Phasing” (Airlie McCoy, Charles Ballard)

The special issue is on schedule for November.

6. CCP4SW and Ligands (Paul Emsley)

The outline program was presented and includes on day 1 crystals to ligand complex structure and on day 2 everything beyond, including validation. There are two introductory talks planned and two on sample preparation, followed by talks on refinement and ligand fitting. There was a discussion as to whether refinement and validation can be summarised, particular in vision of the fact that the programme is quite dense and presently contains too many talks. Preference was given to longer talks and reducing speaker numbers (over fitting all talks in by reducing time slots). Time constraints must be met allowing for sufficient break time and close of the meeting for dinner to allow people time between the last talk on day one and the conference dinner. Further timings must allow time for the popular lunchtime bites, which will be organised different to this year’s with a maximum of two speakers per session. DB proposed to include post translational modifications of proteins; ITE particular with respect to more accessible use of eukaryotic expression systems. JD: a round table at the end of the meeting would be desirable; DB: agree, but unlikely to be well attended on Sunday. The more detailed discussion on topics and speakers is not covered in the minutes. Potential speakers to be invited after this WG2 meeting.

7. **AOB**

The suggestion was made that the next WG2 meeting should target the communication with users, including website, newsletter, etc.

8. **Take note of the date of the next meeting.**

Possible date is September / October (suggested date: 30.9.2015), Locations suggested: London.

9. **CCP4 Gui2 (Andrey Lebedev, Dave Brown)**

CCP4i2 nears completion. What is required for implementation?

The Gui2 timetable for **rollou**t given by Martin Noble in the WG2 meeting in January was:

- alpha as new scientific capabilities scope freeze:1-2 month
- function freeze beta 1 month
- code freeze one further month to fix bugs

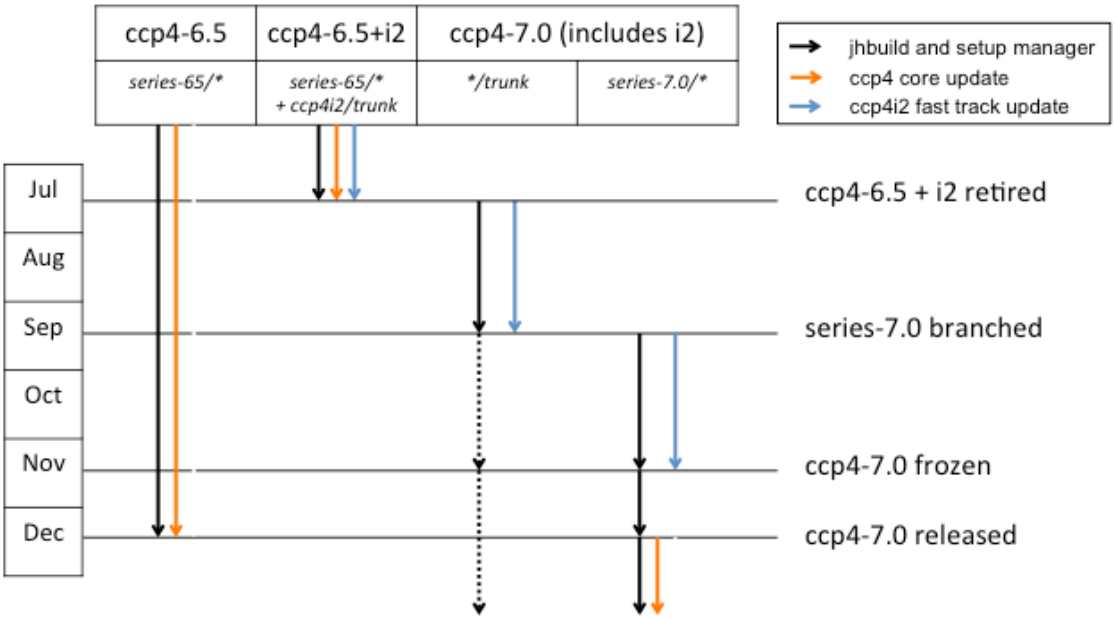
AL demonstrated what was required for the Core group to meet this scheme.

The final additions before scientific capabilities scope freeze would be met with core activities to include python bindings (ccp4srs, clipper) and programs (dials, pdb-redo, shelx) into trunk and builds. This then leads to alpha release as branched series-70, which includes Gui2 (September).

The final changes before function freeze would be met by the core team with an extension of the test system and a tuning of new components, leading to the code freeze beta (September and October).

Core would then require at least a month for bug fixes and general release (November).

An idea could be to have general release coincide with the DLS-CCP4 workshop (December).



This proposal was discussed and accepted. It was clear that requirements for end-users (stable version) are different from the ongoing requirement for developers (quick updates and test environment). It was thus agreed that ccp4-7.0 test binary bundles will come initially from the nightly builds (before the series-7.0

branching point). They would after the series-7.0 branching point come from series-7.0 builds, with bzr update operating form the corresponding branch (initially trunk, later from series-7.0).

The test binary bundles will be distributed a custom setup manager, which will be downloadable through ccp4 + i2 download page. During the release, the updates of both ccp4 core and ccp4i2 will use the standard ccp4 update route.

10. CCP4 Gui2 demo (Jon Agirre)

There was a demo of functionality of Gui2 with user participation, which went very well. Additionally, Jon was presenting video introductions to Gui2 functionality. These received very positive comments and it was agreed to continue exploring options to use these for introductions / tutorials.

During his presentation, Jon focused on the new features that have been introduced since the last WG2 meeting in London (October 2014).

Reworked presentation style

Following suggestions at the Coseners Developers meeting, the use of colour, tooltips and item grouping has been introduced to an apparently very good reception from testers. This was demoed for the Autobuild pipeline. The changes comprise:

- A subtitle widget coloured in blue, which also offers complex tooltips that can be formatted in HTML. This allows for easy sectioning of the tasks and introduces the user to the functionality offered in such sections.

- A separate rectangle coloured in pale yellow with a CCP4 logo with the information that is always present in all tasks, namely task title and follow-up information.

- A new, more visible gradient-based highlighting of errors and incomplete sections in the tasks

Simplified interfaces

It is easier to import MTZ files now, with a mutually-exclusive selection of the column set that can be imported. Also, the project creation task offers a default place for the projects and this speeds up the process, since now you can just specify the new project's name and go ahead.

Native rvapi reports

The pipelines Crank2 and SHELXcde previously used non-native i2 reports (CCP4 online reporting engine, rvapi), and inconsistencies were repeatedly flagged during alpha test. Martin Noble came up with the idea of having rvapi produce XML that i2 can read and interpret. Eugene Krissinel implemented this, Liz Potterton adapted i2 to watch the new XML file, Stuart McNicholas is upgrading the graphing system to match rvapi's and Jon Agirre produced a generic report generator from rvapi's XML to HTML5+JS. While testing is in progress, this is already functional.

Interruptible jobs

It is now possible to settle for a partial solution (e.g. FOM is high enough during DM, or %pct of structure built is high during model building) during the execution of a pipeline and jump into the next step. This was demoed for crank2.

Standardised reports

More clear and with more information. This was demoed for the Autobuild pipeline.

Clipper-python module for crystallographic computing

This was introduced as a way of supporting i2 with crystallographic functionality that can be used and tested without relying on binary updates, speeding up the testing process.