



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 2nd March 2016	Time: 11:00 – 16.00
Location:	Birkbeck, University of London, room 612 Malet St (entry from Torrington Square)	
Circulation:	ccp4wg2@stfc.ac.uk	
Present:	Jon Agirre (JA), Charles Ballard (CB), Dave Brown (DB), Judit Debreczeni (JD), Eleanor Dodson (ED), Paul Emsley (PEM), Richard Gildea (RG), Mike Hough (MH), Nick Keep (NK), Eugene Krissinel (EK), Andrey Lebedev (AL), Ed Lowe (EL), Stuart McNicholas (SMN), Garib Murshudov (GM), Harry Powell (HP), Andrew Purkiss (AP), Christian Roth (CR), Paul Rowland (PR), Khushwant Sidhu (KW), Roberto Steiner (RS), Kyle Stevenson (KS), Ivo Tews (ITE), Julie Tucker (JT), Ville Uski (VU), Melanie Vollmar (MV), Keith Wilson (KSW)	
Apologies:	Arnaud Basle (AB), Kevin Cowtan (KC), Phil Evans (PRE), Vilmos Fulop (VF), Ronan Keegan (RK), Karen McIntyre (KM), Rob Nicholls (RN), Jose Trincão (JT), Johan Turkenburg (JPT), Graeme Winter (GW), Marcin Wodjyr (MW)	

Please arrive for coffee at 10:30.

Directions <http://www.bbk.ac.uk/geology/contact-us/how-to-find-us>

1. Approval of minutes from the Cambridge WG2 meeting 30/9/15
2. Chairs report (Ivo Tews)
3. CCP4 SW2015 “Phasing” Acta Cryst Proceedings Issue (Charles Ballard, Airlie McCoy)
4. CCP4 SW2016 “Protein-Ligand Complexes” (Dave Brown, Judit Debreczeni)
 - a. Digest / Feedback
 - b. Plans for the Acta Cryst Proceedings Issue
5. CCP4 SW2017 “From Crystals to Structure” (Ivo Tews)
 - a. Programme
 - b. Potential Organisers

Lunch

6. CCP4 SW2017 appointing organizing team (vote)
7. What’s New in CCP4 Core Group, CCP4 7.0 (Eugene Krissinel)
8. Gui2 (Jon Agirre)
9. DIALS (Richard Gildea)
10. CCP4 online (Ville Uski)
11. Conferences and workshops (Charles Ballard)
12. Web pages (Eugene Krissinel)
13. AOB

Take note of the date of the next meeting (proposal 8.6.2016)

16:00 close

Minutes

1. Approval of minutes from the London WG2 meeting 30/9/15

The minutes from the London WG2 meeting 30/9/15 will be circulated by mail to WG2 and subsequently put on the web.

2. Chairs report (Ivo Tews)

The main topics going forward in the previous year, both in CCP4 WG meetings and in developers meetings, were Gui2, ligands and DIALS. The upcoming 2017 study weekend "From crystal to structure" (put forward by WG1) is therefore a timely opportunity to feature these topics, focusing on use of Gui2. Reviewing the series of study weekend topics, this follows on in cycle from last covering this topic in 2010.

The feedback on release of CCP4 7.0 including GUI2 is sparse. It would be wise to gather further feedback on use of the software.

DIALS was released along with CCP4 7.0. This could, in logical continuation, lead into a data-processing focused SW2018 which was last featured as a study weekend topic in 2012. This meeting would also feature emerging and more widely used multi-crystal techniques.

Study weekends are popular, and over the past years we have seen an increasing interest with a higher number of registrations. It would be feasible to plan future meetings with a 10% increased registration number. One would have to set this against the logistics of the venue.

The WG2 remit is defined as being constituent form users of the software, thus this group provides a good forum for getting feedback. It would still be advisable to tie this in with heavy crystallography users, such as present in DLS BAGS. Efforts to gain membership through a general call by mailing form DLS have had little effect in getting new members and must be continued.

3. CCP4 SW2015 "Phasing" Acta Cryst Proceedings Issue (Charles Ballard, Airlie McCoy)

The SW2015 papers are out in the March edition of Acta D.

The discussion focused on what would constitute a good Acta D/Study Weekend article. There was a feeling that the editorial processes, lead by the study weekend organizers, could better identify review and research type articles, giving some more flexibility in the reviewing process. This would help refereeing. A decision on the process requires confirmation with IUCR.

4. CCP4 SW2016 "Protein-Ligand Complexes" Digest, Special issue (Dave Brown, Judit Debreczini)

Meeting was well received all round. WG2 commend Paul and Judit on the organisation of the study weekend (DB, seconded ED). It was noted that attendance was good until the end of the meeting.

There was a strong, shared feeling that the study weekend had the desired educational tilt. It was discussed whether this meeting on ligands in deposited structures goes back to the lab to change practice (DB) and would then eventually lead to improved depositions. It was also noted that there is a "ligands task force" (Ligands Group) that identifies problems and have an effect and influence the quality of structure depositions in future years.

Speakers were encouraged to speak to each other, avoiding duplication (RS). Streaming of talks was again seen as a very useful feature (NK). Some of the talks might have benefited from more time (DB).

Problematic – as often – were the lunch-time bites, when they were overrunning. There were also Issues with queues for serving of food impacting upon students attending the lunch-time bites. Options discussed were limiting general attendance to the study weekend, changing the number and cycle of lunchtime bites, introducing bar-bytes in the evening, or even the main program. No “easy” solution was identified, and the topic needs to be discussed further.

The topic “what is my blob” might not have been fully covered by the study weekend, may be pointing at a lack of automated interpretation procedures in the CCP4 suite (PE). There would seem to be a need for tools that will take prior knowledge and apply this to any undefined density (AP). There was a useful discussion around this calculation and decision of what the electron density **is** remains a problem (DB). It was suggested this could be addressed in the editorial of the proceedings issue to tie talks together.

The current plan for the Acta D proceedings issue was presented (JD), which, so far, is a long list of intentions and a good cover of the meeting. Publication ideally occurs close to the meeting (otherwise it will be forgotten), but clearly the time target must be to have the issue released by the upcoming study weekend (ITE). There was a discussion whether articles that are revised / accepted can be made available before the publication of the special edition, which we will explore for future issues.

5. CCP4 SW2017 “From Crystals to Structure” potential programme and organisers (Ivo Tews)

The topic from “Crystals to structure” was suggested by WG2 in September and put forward to WG1 and ratified. The scope of the meeting will have to be clearly defined. It offers an opportunity to promote i2 but will support the whole of the CCP4 suite developments. The focus of the study weekend is on the core structure solution process, and will have a chance to include “modern” methods. Organisers of this meeting would be open minded and fit / shape these programming requirements. The programme is to be further discussed in the next WG2 meeting in Summer. A few points of the discussion:

- Experimental Phasing, Molecular Replacement and Model-building and Refinement
- There must be something on where the crystals come from, and this could be an intro talk
 - Testing crystallisation success, e.g. in-situ? VMX suggested by (DB)
 - Crystal engineering (RS)
- More on validation, less on sample preparation. (JD/GM)
- Is crystallography getting easier? (IT)
- Using Prior knowledge: is the target unique or novel (in terms of fold) - i.e. is MR a potential path for structure solution? (DB)
- Some focus on structure analysis, e.g. prosmart, PISA ... (GM)
- Using complementary methods information in crystallography, eg. data from EM, NMR ..., or the other way round when crystal data is used from EM (EK).
- Consensus: focus on core practices, but extend to include, e.g., validation, modern methods, multi-crystal techniques.
- Looking forward, DB and GM suggest that “data processing / multi-crystal” would be timely for the next meeting.

As each meeting gets its own proceedings it is a major opportunity. It serves as a reference point for the CCP4 suite, similar to the NAR database issue for that community. It marks a point in time, and is a good opportunity for developers to publish and update / rejuvenate these key reference papers for their software. The organisers of the study weekend have to have oversight on this as they will edit the special issue.

- Publication of articles is also critical for grant renewal (DB).

The present plan is to repeat lunchtime bites on both days, and look into ways of improving the overlap with lunches. There may be an opportunity to add bites in the evening. We will use all available rooms for bites (VU to take note), but only have one topic in each room.

6. CCP4 SW2017 appointing organizing team (vote)

DB suggested KM as organizer; IT suggested MH as organiser. WG2 selected KW and MH as organisers.

7. What's New in CCP4 Core Group, CCP4 7.0 (Eugene Krissinel)

CCP4 7.0 released on 6 Jan 2016, with the Windows version released one month later.

The new features of CCP4 v.7 are release of Gui2 as well as inclusion of DIALS, SHELX, ARCIMBOLDO and molprobit (several features, with work going on for full integration). The release was smooth; some pressure resulted from last minute changes and failure to have a code freeze in place.

The windows release was delayed with compile and port problems, particularly with sophisticated components and graphics. Issues in the windows platform became apparent at the Indian workshop. These were mainly memory demands, as there are issues with the 2Gb memory limit on 32-bit windows; these problems may not easily be resolved.

Changes to update policy. CCP4 6.5 used a non-intrusive prompt, CCP4 7.0 now prompts the users. Conservative estimates suggest that 70% of all users never update, and this has not changed much since introduction of the new policy. There is a discussion about automatic updates.

Kyle Stevenson is introduced to WG2 as the new core group member for Windows.

8. Gui2 (Keith Wilson, Jon Agirre)

The new Gui2 is included in CCP4 7.0. The functionality is good now, and Gui2 has solved some structures that were not easy to solve in Gui1. Positive feedback was received at workshops. The addition of tutorial and help material is another good feature. Demo data on easy problems are provided.

Technical issues include addressing of memory in 32-bit Windows (unresolved), running over NFS where Gui2 can become slow, and remote launch of jobs. Progress is being made on transferring projects from i1.

Experienced users miss some advanced functionality in Gui2, and this may lead to switching back from Gui2 to Gui1, which are cases developers need to catch.

In contrast, some feedback has indicated the phaser-MR tasks are too complicated. Also, for long tasks like phaser, there is no output for a long time while the job is running, and intermediate running reports would be nice.

A new feature is the export functionality that will allow exporting reflection and coordinate files to a given name (overcomes problems with them calling XYZOUT).

A video was shown on use of Gui2. Jon demonstrated how the ccp4gui2 interface can view/import data from a ccp4i project (nice drag and drop of data); he demonstrated further gui2 tasks e.g. clipper python job for b-factor analysis. Further remarks:

- Job rating is regarded as a plus (IT)
- progress on running job, and output produced during – the running man is too little of an indicator for progress (IT)
- there were not many comments on ccp4bb on use of gui2 and 7.0
- some of the feedback centered on (insufficient capability) of gui1 import into Gui2 (EK)

It was suggested to feature Gui2 at the developers meeting in March and in the next WG2 meeting.

9. DIALS (Richard Gildea)

Richard reported on developments and updates from DIALS. The reciprocal lattice viewer was described as *the* powerful tool. Experiences with interfacing with Chemical Crystallography (I19) were reported. Richard proposed to make a rogues gallery of problematic indexing datasets available.

10. CCP4 online (Ville Uski)

VU presented a “quick” run through ccp4online, in particular the new pipelines, and plans for the CCP4 cloud implementation.

11. Conferences and workshops (Charles Ballard)

Workshops were held in China, Japan, and in India, the latter identifying problems with the 32bit Windows release. The CCP4/DLS Workshop in Harwell was used as a test for ccp4i2 use, leading to some last minute identification of bugs that helped release in January.

12. Web pages (Eugene Krissinel)

For the new CCP4 Website design, STFC/SCD has now a suitable program for the support of SLA CCPs, a centralised facility for providing websites. The website will be a virtual machine running drupal. They will provide this for CCP4 and CCP4EM, but a lot of effort will be required for transferring contents (unresolved).

13. AOB

The WG2 group thanks Harry Powell for his contributions to CCP4 over the past years and wishes him well.

14. Take note of the date of the next meeting.

Agreed 8.6.2016, London.