



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 12th July 2017	Time: 11:00 - 16.00
Location:	Birkbeck, University of London, Seminar room 612 (entry from Torrington Square)	
Circulation:	ccp4wg2@stfc.ac.uk	
Present:	Charles Ballard (CB), Mike Hough (MH), Ronan Keegan (RK), Eugene Krissinel (EK), Karen McIntyre (KM), Andrey Lebedev (AL), Stuart McNicholas (SM), Luis Fuentes-Montero (LM), Rob Nicholls (RN), Arwen Pearson (AP), Khushwant Sidhu (KS), Kyle Stevenson (KyS), Ivo Tews (IT), Ville Uski (VU), Melanie Vollmar (MV), David Waterman (DW)	
Apologies:	Arnaud Basle, Kevin Cowtan, Ed Lowe, Robin Owen, Paul Rowland	

11:00-16:00 WG2 agenda

1. Approval of minutes from the DLS WG2 meeting 15/2/17
2. Chairs report (Ivo Tews)
3. CCP4 activities, workshops and courses (Charles Ballard)
4. Acta Cryst Proceedings Issue "From Crystals to Structure" (Mike Hough, Charles Ballard)
5. Planning of the CCP4 SW2018 "Multi-Crystal and Data Collection" (Ivo Tews, Arwen Pearson)
 - a. Proposed draft programme
 - b. Proposed speakers and chairs
 - c. Plans for the Acta Cryst Proceedings Issue
 - d. Organisation of the meeting, Lunch-time-bytes (Charles Ballard, Ville Uski)
6. Outreach and Teaching, CCP4 grant proposal (Ivo Tews, Charles Ballard)
7. DIALS - News and on-going development (David Waterman)
8. DIALS GUI - Development and Demo (Luis Fuentes-Montero)
9. Take note of the date of the next meeting (proposal 27. September 2017)
10. AOB

We will break for lunch during the meeting.

Minutes

1. Approval of minutes from the DLS WG2 meeting 15/2/17

The minutes from the DLS WG2 meeting 15/2/16 were approved.

2. Chairs report (Ivo Tews)

WG2 is to oversee organisation of the study weekend. We have now appointed Arwen Pearson, Robin Owen and Max Nanao as Organisers for the SW2018 “Multi and Serial Crystal Data Collection and Processing”.

Activities of the WG2 chair over the past period included some exploratory work on documentation and teaching (courses, tutorials). IT gave a short presentation at the developers meeting that was held in March 2017 at Cosenser's. A number of ideas are being discussed:

- Maybe in a DropBox/One Drive type solution for teaching materials and tutorials
- AP suggested using existing Wikis; it was pointed out by core that there are restrictions (storage etc.)
- RN suggested could store behind the CCP4 website in a private area or in CCP4Forge
- Also: needs to address how we archive and update documentation and manuals/resources
- RN points out that i2 documentation should be provided at the same place as general CCP4 documentation. CB points out this can be hosted anywhere (transparent to the interface)

The new CCP4 web pages are work in progress and now being drafted up in a WordPress version, outsourced to STFC Media Services. The advantage is easy editing by selected users. The plan would be that WordPress is front end to VM's and proxies behind.

How all this ties in with CCP4 activities and the next grant proposal planned for 2018 is discussed under (6).

3. CCP4 activities, workshops and courses (Charles Ballard)

CB reported on meetings: the ACA, New Orleans, USA, and IUCr, Hyderabad, India; workshops: CCP4/Institute Pasteur South American School, Montevideo, Uruguay, 2017, 20 students; CCP4/Phenix, Hyderabad, CCP4, Guangzhou, China. 23-27 October 2017, 20 students; CCP4-DLS, November/December 2017, 20 students; workshops and conferences where CCP4 is invited guest: AL: Rapiddata, Stanford, April 2017; DW+AL: Oulu, Finland, May 2017; EK: Madrid, Spain, May 2017; DW+AL: Electron crystallography, PSI, September 2017; CCP4 sponsored conferences: SWSBC meeting, Cardiff, July 2017, Northern Structural Biology meeting.

- RK reports from APS: ~10 new structures solved; observation that students at APS schools know about CCP4 before, not just Phenix
- A one-day CCP4/Phenix meeting is to be held before the IUCr conference
- The CCP4/DLS workshop keeps to be 4x over-subscribed
- CCP4 demonstration held at the SWSBC meeting over lunch, but needs better timing / advertising
- SID: The Northern Structural Biology meeting (Carlisle) would benefit from higher attendance numbers and needs better advertisingA

Conclusion: conferences and workshops raise the CCP4 profile and reach an international audience.

CCP4 core activity is release of CCP4v7.1. This is awaiting finalisation of integration of Molprobit, Whatcheck, PDB-REDO, Dials DUI, and Auspex and currently anticipated before x-mas this year.

4. Acta Cryst Proceedings Issue “Crystal to Structure” (Mike Hough, Charles Ballard)

We are on track presently with submissions. Against the meeting with 23 talks, a total of 20 articles were anticipated, two of which have been merged leading to a total of 19 articles for the special issue.

The current stats:

- 1 accepted
- 11 have the review completed and are in revision
- 4 submitted and under review
- cut-off date end of July for any remaining submissions

It was discussed whether the special issue represented the breadth of the meeting, and covers the topic from crystal-to-structure to serve as a reference for the coming years before this topic comes up as SW again. It was felt that the article on i2 is essential, and an update on refmac and on coot would be nice.

Publication of the special issue is planned in two issues in December 2017 and January 2018.

5. Planning of the CCP4 SW2018 “Multi-Crystal and Data Collection” (Ivo Tews, Arwen Pearson)

IT: The study weekend has a clear motivation, as we have seen monumental changes to data collection and changes to samples. In the times of automatic collection, we should give guidelines to re-processing data. Fins slicing and noise free detectors mean that images are very pale, challenging teaching. Ever-smaller samples make radiation damage integral to the data collection process, and change sample delivery. We are currently seeing a tendency to automated data acquisition and processing, and random shooting (scanning) of grids where crystals are not even visible. All changes the way we look at data processing. The special issue coming from this meeting should capture this change in culture and be a reference point going forward. Speakers should be able to teach best practice, talks need to be didactic.

AP: will change the title to "Multi- and serial-crystallography data collection and processing". The structure of the meeting could be day one giving “background and experimentation”, while day two focuses on software. The following sessions are anticipated:

- Session 1 – Introduction and Overview
- Session 2 – Need for Multi and Serial Measurements
- Session 3 – Sample Preparation and Getting Crystals into the Beam
- Session 4 – Processing multi crystal and serial data
- Session 5 – Phasing, Refinement and Validation
- Session 6 – Future Perspectives

The current list of proposed speaker includes 25 names, of which six are female, six to seven are transcontinental, and nine to ten are EU.

IT: Gender balance, also need to restrict transcontinental for keeping the costs of the meeting in check to not have to change registration fees. However, there is a way to keep costs for transcontinental speakers in check by adding a section into the speaker’s invitation letter to state that CCP4 will arrange travel to avoid late bookings and/or expensive fares. The speakers for the introductory talks proposed are good as these are known to give good and didactic talks. The overall number of speakers is (too) high for a two-day meeting, a total of twenty talks are more appropriate not to have to rush through the programme and go over the attention span of the audience. The program committee should make use of the offer that different talks can have different durations. Also note that we need to keep eye on the Special Issue having a good spread of topics and representing the meeting well.

RK: could add Electron Diffraction (DW suggested a good female speaker for this)

MH: cover the future and include talks on XFEL/MXFEL

CB: include MAX4 microfocus

MH pointed out overlaps between talks; AP: some of these are on standby and hence the total number of speakers invited may also reduce.

IT: is it wise to have the processing session that is theory heavy first thing on day two? AP: this was discussed at length in the organising committee and felt to be the natural place and best to be programmed this way. Others seconded and said this session, because of the importance, will find good attendance.

It was discussed and felt that up to 2/3 of all talks might report applications. Possible cuts in the presented programme discussed were on sample handling, as well as merging and processing.

It was unanimous that DIALS is central to the meeting; Suggestions included to present DIALS in relation to the multi-crystal topic, e.g. a multi crystal profile model and maybe scaling?

The programme was approved.

Organisation of SW2018 (CB/KM/VU)

Suggestions for the What's New in CCP4 session discussed were: Lorestr, DUI, Auspex; base around Gui2.

The lunchtime-bytes were successful and sought after as ever. Particularly, DIALS and BLEND sessions were full. People seemed to be happier with the SW2017 format of one byte per room per day (as supposed to the SW2016 format with multiple talks). The format for SW2018 will therefore be one talk per person per room.

Some topics oversubscribed; it was discussed whether people should sign up on the day but this was dismissed; instead intelligent programming should prevent oversubscription, learning from experience, e.g. by offering DIALS sessions (one of the oversubscribed topics) in larger rooms (not ideal) or offer them twice either simultaneously in different rooms or on different days.

After demand from delegates, it was discussed whether we would be able to introduce a networking event to be held in parallel to the WG1 speakers dinner. The event would cater to students coming on the evening before the meeting starts so they can attend "What's new in CCP4?" on day one at 9 am. The event would take the format of an informal gathering for networking purposes, should be open and free with food such as pizza / chips / puddings (tbd) and a cash bar. IT: CCP4 Exec in favour.

The networking event was approved by WG2.

6. Outreach and Teaching, CCP4 grant proposal (Ivo Tews, Charles Ballard)

CCP4 has requirement and offers documentation on software for three purposes: developer's documentation, documentation for users, as well as tutorials and lecture materials for conferences / workshops / demonstrations / self-taught tutorials. Further, CCP4 requires and offers Web pages that give access to programs and documents, as well as course materials. A scan of the available resources has shown that materials are scattered and could benefit from better structuring in the presentation. There is an identified need to collate all information in one place, so it is readily available for the relevant people to use.

With respect to the user documentation, CCP4 received an enquiry whether we could re-issue and update a pdf-type CCP4 manual. This was discussed, and while it is difficult to see whether anyone would be volunteering to take on such a task, there is also on-line help (e.g. within Gui2) which was felt to be generally of good standard. In terms of offering a manual, it was discussed that well executed and available tutorials would be an alternative for teaching the software (learning-by-doing). To be revisited in the next WG2. This information should migrate to the CCP4 webpages (single location).

CCP4 grant proposal 2018

IT: WG2 generates impact, and this needs to be harvested and should be reflected in the grant via strategic goals. Presentation of a proposal that links some of the key functions of the WG2 to the BBSRC grant application in order to add to the Impact Summary. This points out the active user community and the structures supporting this that are already established, such as CCP4BB and WG2 as user platforms.

MH/AP: include impact from all areas including conferences etc.

EK: was of understanding that impact in grant applications related only from scientific impact.

AP: Impact is not only scientific; indeed, funding agencies specifically request an impact section along the described lines. Good to make it explicit in the grant proposal.

MH: the time commitment must be concrete rather than voluntary as is at present.

CP: Problem of putting money against these goals as we are close to the £2M ceiling on developer funding.

RK: suggest outsourcing.

AP: queried whether could have Industrial Funding contributing to this.

AP, MH: volunteered to help with wording.

7. DIALS – News and on-going development (David Waterman)

DW: Short presentation on functionality and development of the DIALS software.

8. DIALS GUI – Development and Demo (Luis Fuentes-Montero)

Demo of the GUI: runs using the iDIALS backend. Report on updates implemented following suggestions from WG2 after the last presentation. There was a major change required after the philosophy of navigation has changed. Critical issues before Dec release: Masking backstop shadow and automatic running static then varying refinement. Not essential (but nice) for release are a Reciprocal lattice viewer (use Marcin's Javascript viewer). It was discussed whether an auto-advance step should be contained. The update was warmly received. Further suggestions:

AP: import icon looks like "exit". Perhaps use an arrow icon? The values for the models beam, crystal, detector etc. should be editable? Should the refine_bravais_setting step lead with cell dimensions first, not the delta? To compare, iMosflm puts lattice type first, penalty, cell, rmsd, nref, delta beam. Also: Make more obvious which is the recommended solution.

SM: Colour-blind palette needed.

Further: Refine: should do static first then scan-varying second always by default. Guidance for the user ("Click the Dials icon to run >> refine") might be better under the Stop and Dials buttons rather than right at the bottom. Search string in advanced parameter is very good! Can we have a 'find next' button to scroll down to each match? Image viewer needs a detach button to pop that window out. GUI to accept a state file argument rather than just restarting in a directory. Then user can double-click on a state file to launch GUI. File->Open should allow opening a previous state. Stuart: Would need that form of launching GUI in order to work well with ccp4i2. Allow choice between multiple state files in a directory when launching. Swap Go and Stop buttons round (stop on the right), make buttons the same size, grey stop out unless it is possible to press it (when a job is running).

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

Possible date 27.9.2017, Location: DLS or London. Google poll to follow.

10. AOB

None.