



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 20 th January 2021	Time: 14:00 – 16.30
Location:	zoom	
Circulation:	ccp4wg2@stfc.ac.uk	
Attending:	Jon Agirre, Svetlana Antonyuk, Charles Ballard (CB), Arnaud Basle, David Briggs, Ivan Campeotto, Atlanta Cook, Kevin Cowtan, Eleanor Dodson (ED), Paul Emsley (PE), Maria Fando, Ralf Flaig, Vilmos Fulop (VF), Jonathan Grimes (JG), Mike Hough, Misha Isupov (MI), Robbie Joosten, Ronan Keegan (RK), Nick Keep, Eugene Krissinel, Oleg Kovalevskiy (OK), Andrew Lebedev (AL), Ed Lowe, Airlie McCoy, Karen McIntyre, Stuart McNicholas, Garib Murshudov (GM), Ro Nicholls (RN), Nick Pearce, Anastassis Perrakis, Andrew Purkiss, Alan Roseman, Pietro Roversi, Paul Rowland (PR), Roberto Steiner (RS), Kyle Stevenson, Ivo Tews, Ville Uski, Melanie Vollmar (MV), Keith Wilson, Marcin Wojdyr	

5 mins breaks at every full hour

1. Approval of minutes from the WG2 meetings 24/09/20
2. Chairs report (Ivo Tews)
3. CCP4 – core group news (Eugene Krissinel, Charles Ballard, Kyle Stevenson)
 - a. Updates and news
 - b. Documentation
4. SW2021 digest (Charles Ballard, Ronan Keegan, Ville Uski, Ivo Tews)
 - a. Participant numbers
 - b. Feedback (please all contribute)
5. SW2021 digest (Atlanta Cook, Dan Rigden, Anastassis Perrakis, Randy Read)
 - a. Acta D Special issue
6. Future of CCP4 offerings (Charles Ballard, Keith Wilson, Ivan Campeotto)
 - a. the Study Weekend plus, workshops and schools, developers meeting, local meetings, roadshows
 - b. Local meetings: Northern
7. SW2022 prep, working title "refinement" (Ivo Tews)
 - a. Topic
 - b. Format
 - c. Appointing organisers
8. Take note of the date of the next meeting (proposal 17th March 2021)
9. AOB

Minutes

1. Approval of minutes from the online WG2 meeting 24/9/20 (Ivo Tews)

The minutes from the online WG2 meeting 24/9/20 were approved online.

2. Chairs report (Ivo Tews)

The organisation of the CCP4 online study weekend took additional time and required organisation of a number of technical meetings that ran in the background, outside the WG2 group. Consequently, the Study Weekend webpages took longer than usual to iron out some uncertainties, but this seemed not to have been to the detriment of registrations.

The new CCP4 webpages are a success. Feedback is always welcome, but so far there were no serious complaints which is taken as a good sign. Some legacy items still need to migrate. Good would also be to obtain usage figures (VU to install plugin) to optimise usability.

It was also decided (at EXEC) to update the membership of WG1, to be actioned.

3. CCP4 – core group news

a. Updates and news (Charles Ballard)

CCP4 Release 7.1 is out. There is a monthly update schedule. This is the last release that will contain support for Python2. Ongoing updates include cloud and monomers, and the i2 docs are now on github. CCP4 core awaits arrival of M1 Macs for testing. CCP4 7.1 is gradually replacing 7.0, which still sees quite a lot of usage.

The next release will be CCP4 8.0 which then fully supports Python3 with pyside2, and this release will require considerable testing. The release will include an updated i2 and ccp4mg, planned are DIALS3 series and PDB_REDO. There are presently issues with Windows as the QT Web-engine is not supported. Linux and Mac binaries are available for testing, please contact CB.

CCP4 Online has moved to STFC/cloud/IRIS. The increase in available resources over the ccp4 machines is 12 x 16 VCPU + 48GB. Presently, 8500+ jobs run with 800+ active users.

CCP4 Cloud was used in the DLS/CCP4 workshop in conjunction with STFC Cloud w/o problems. Development continues on stability for a growing user base, new interfaces, and on user assistance; there are presently 1200+ registered users.

b. Documentation (Kyle Stevenson)

Documentation is available online and offline through CCP4i2. The latest version has dropdowns and is now easy to edit. You will need a Github account; please send KS e-mail with username for permissions. KS demo'd editing in .rst format. An e-mail to the CCP4 Developers group went out. CCP4i2 is nearly finished; this is an organic process where everyone can get involved with editing/updating their sections. Most of the old documentation has already been ported.

4. SW2021 digest (Charles Ballard, Ronan Keegan, Ville Uski, Ivo Tews)

The SW2021 as a fantastic meeting. It was Brave to take on an online meeting knowing what's at stake and be successful! CCP4WG2 thank Atlanta Cook, Dan Rigden and Anastassis Perrakis!

a. Participant numbers

The online meeting has been beating our records, we had over 1800 registrations. The attendance in the individual sessions was between 400 and 700, and thus higher than in any previous CCP4 meeting.

What's New was very popular, and about three times as many people attended than usual.

Lunch Time Bytes overall ran quite well, and averaged 30/40, which is more than in previous years. On the 1st day, Refinement and DIALS were most popular; on the 2nd day, Arcimboldo, Conplot and PDB offerings took the main attention; on the 3rd day, Coot, ShelX and CCP4i2 were most popular. People seemed to like the anonymity of the chat function as many questions were asked; while this is so, it would be useful to have a 2nd person to moderate the chat and ask the question to make this easier for the presenter.

The DLS MX User meeting attendance was also double from previous. People who attended DLS meeting were those UK Users. Ralf Flaig (DLS) appreciated the use of the online platform but commented the user discussion / interaction was lacking. The link with the CCP4 Study Weekend, however, was seen as an advantage.

b. Feedback

An online meeting, in principle: should be easier to organise; play to the advantage of EDI; is cheaper; can get more speakers and from further afield; attracts more attendees; has the advantage of talks and content being seen online and offline. The question is: does it replace a real-life meeting? An online meeting does lack personal quality and falls down on interaction and chance meeting of similar minds. The length of the conference days (half days) and sessions (2 hrs) and duration of the conference (4 days) was about right.

Problems: Because of the organisation behind this online conference, on the fly changes were easy; while there were some glitches these were fixed quickly, and requested changes were implemented. Thanks to Laura and Stuart.

The Q&A sessions could have been more effective and have overall seen too little traffic in the individual speakers' rooms; to test, we changed this for one session and a moderated Q&A seemed to have worked better. A way for continuing discussions – e.g. Slack/Discord – would be a good idea for the future, but would need to be integrated into the online-platform.

The challenges ahead in 2021/2022 to do more online meetings and learn from experience and improve discussions and interaction. A number of different and new elements are needed:

- Interactive elements
- stimulate discussion across age/experience
- raise interest across themed rooms
- identify new talent
- have different social events and motivate participation in online socials

To address this in future, we would possibly have to match a social organisers team and with the scientific organisers.

MV: an idea could be to randomly place people in a room together to find out answers to set questions, with shuffling of teams during this event.

5. SW2021 Special Issue (Atlanta Cook, Dan Rigden, Anastassis Perrakis, Randy Read)

The study weekend had 43 speakers. The scientific organisers have sent letters out to remind speakers of the requirement to publish in the proceedings and have agreement from all but two that were asked. As the special issue should deliver about twenty articles, there is scope for collaboration and shared authorships, and this is being explored.

Next steps: end of April submissions is expected, and reminders for contributions will go out, however manuscripts must be in by June to give appropriate time for review.

6. Future of CCP4 offerings

a. the Study Weekend plus, workshops and schools, developers meeting, local meetings, roadshows (Charles Ballard, Keith Wilson)

CCP4 offers the study weekend, the developers meeting, local meetings and roadshows. The next SW2022 is proposed with F2F where possible; this may be a hybrid meeting, i.e. the meeting will be open for attendance for both F2F and via virtual hub. The developers meeting is in July at Cosener's as F2F; the option is to convert to a virtual event if necessary. Proposed is that at least one WG2 meeting is F2F but others are held virtually, which should open up to a wider audience.

The schedule of meetings and workshops has of course been impacted by COVID. Virtual were / are: the DLS workshop Dec 2020, the SW2021, the South Africa Feb-March 2021, and APS in Summer 2021. Not decided yet are SEACOURT, Thailand (autumn 2021), South America (Sept 2021), DLS (Nov/Dec 2021), and the SW2022 (Jan2022, Nottingham).

b. Local meetings: Northern (Ivan Campeotto)

The Northern Meeting has not yet been re-established. It can take some recent experience from the South Western meeting which was held online in 2020, and runs annually (SWSBC) with a rather stable 70-110 attendance that is focussed on junior lab members and ECRs. To reactivate the Northern meeting IC contacted PI's at other Universities to gauge their level of involvement. So far it is not entirely clear whom to include, but the query is out for members between Leicester and up into Scotland; Newcastle and York have already indicated they are happy to be involved. Like SWSBC, the Northern meeting would rotate venue among participating members. IC and KSW will get together to see if it is possible to host the event in 2021 (to report back at the next WG2 meeting).

Further, if this goes ahead there will be scope to also instigate a meeting for the South East.

CCP4 will support any of these undertakings.

7. 1. SW2022 prep, working title "refinement" (Ivo Tews)

a. Topic

The general topic of the study weekend is Refinement, going with the rota of meetings. After input from WG1, the meeting could include / cover refinement, types of data (as in X-ray, EM, Neutron, NMR, spectrochemistry), model completion, validation, deposition.

New boundaries would include multimethod models, modelling of radiation damage, inclusion of time resolution, multi-crystal and multi-state depositions.

b. Format

Planning should be for an on-line meeting, though this might be updated to "hybrid", see section 6a above.

c. Appointing organisers

A number of potential organisers were suggested and discussed. IT to appoint a team of three shortlisted candidates. Report back next meeting.

Organisers will then get together to look at possible speakers; these are to be discussed at the summer WG2 meeting. No promises should be given to possible speakers until ok'd at WG2 meeting.

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

Proposed date: proposal 31st March 2021, online.

9. AOB

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