



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 29 th June 2020	Time: 09:00 – 13.00
Location:	zoom	
Circulation:	ccp4wg2@stfc.ac.uk	
Attending:	Jon Agirre (JA), Charles Ballard (CB), Arnaud Basle (AB), Tom Burnley (TB), Atlanta Cook (AC), Kevin Cowtan (KC), Kay Dietrich (KD), Eleanor Dodson (ED), Tarik Drevon (TD), Paul Emsley (PE), Maria Fando (MF), Ralf Flaig (RF), Luiso Fuentes-Montero (LFM), Mike Hough (MH), Robbie Joosten (RJ), Oleg Kovalevskiy (OK), Eugene Krissinel (EG), Ed Lowe (EL), Stuart McNicholas (SMN), Peter Moody (PM), Garib Murshudov (GM), Nicholas Pearce (NP), Tassos Perrakis (TP), Andrew Purkiss (AP), Dan Rigden (DR), Johann Turkenburg (JT), Sameer Velankar (SV), Melanie Vollmar (MV), Klemens Vonnrhein (KV), David Waterman (DW), Keith Wilson (KSW)	

5 mins breaks at every full hour

09:00-13:00

1. Approval of minutes from January WG2 meeting
2. Chairs report (Ivo Tews)
3. CCP4 Core team news (Eugene Krissinel)
 - a. Cloud (Eugene Krissinel, Oleg Kovalevskiy)
 - b. CCP4v7.1 (Charles Ballard)
 - c. Documentation (Eugene Krissinel, Maria Fando, Ivo Tews)
4. CCP4 activities, workshops, roadshows (Charles Ballard)
5. Experience with online workshops and conferences (Ed Lowe, Tom Burnley, David Waterman)
6. Experience from organising a CCP4SW (Jon Agirre)
7. CCP4 SW2021 “Integrating Structural Biology” (Atlanta Cook, Dan Rigden, Tassos Perrakis)
8. *New Software (scheduled but postponed to July and September meetings)*
 - a. *progress on ED (Tarik Drevon)*
 - b. *Refinement against different experimental targets (Garib Murshudov)*
 - c. *Deposition of multi-method datasets (Sameer Valenkar, John Berrisford)*
9. next meeting: 24th September
10. AOB

Minutes

1. Approval of minutes from the London WG2 meeting 29/1/20 (Ivo Tews)

The minutes from the London WG2 meeting 29/1/20 were approved online, following the meeting.

2. Chairs report (Ivo Tews)

Appointment of the CCP4 SW2021 organisers was delayed bc. of the uncertainty of the meeting format in COVID times. Potential organisers were contacted with the proviso that the meeting might have to be online.

CCP4WG discussed the options that lay before us:

- full meeting 350 attendees
- limited (130 with masks) +zoom +some remote speakers
- limited (RAL) +zoom +remote speakers
- virtual only

CCP4WG2 discussed these options and decided only a full virtual meeting would be viable. Indeed, the organizer appointed in May had received a steer from the WG2 chair that they would have to consider mainly an online option. CCP4WG2 have appointed Atlanta Cook, Dan Rigden and Tassos Perrakis as organisers for the 2021 Study Weekend.

COVID19 caused collateral damage to other meetings and workshops (coming up). The CCP4 sponsored event for the South West, the SWSBC meeting, was initially cancelled. The CCP4WG2 chair then promoted the option of an online event, which was first met with scepticism and then got accepted by the consortium. The SWSBC2020 meeting was then advertised as a collaborative online event between the eight SWSBC consortium partners. The event would include five scientific sessions, two plenaries, a poster session, a social, and a CCP4 Roadshow. ITE and Ed Lowe / Stuart Mc Nicholas will give post meeting report at the next WG2 meeting.

SMN: Will provide a new "Quickstart video".

CCP4WG2 will continue to look at improving the success of the software. This can be done by training (workshops and roadshows, bringing back user feedback to the core team), by querying users directly for feedback and functionalities sought, and by ensuring the software is cited on deposition. Efforts in this direction need to continue and intensify. The new functionalities rolled out with v7.1 mainly around simplifying deposition are a good way to increase citation.

AB: The deposition tool works well and should perhaps be publicised more. This tool has a quality that could convert to using i2 even more. We should support this more actively, for example in a video. A message for all via bb should be posted. We should also think about a publication, e.g. in ActaF. Follow up.

Kevin has past study weekend material that never got published; this is on underlying technologies eg buccaneer; shift field (work of a post doc had left), or a test data – these are generally not followed up because they are not considered interesting, are technical in nature, or are not making a "full" scientific paper. However, this poses the question what should be done with this material, for example as an open archive hosted on the CCP4 web pages, or as publications in the CCP4 newsletter that could be revived and enriched. WG2 discussed this.

GM: This would be published outside ccp4 special issue? It is a good idea but what is it?

DR: Surely, we just continue to publish CCP4 stuff, outside SW issue if necessary, in the usual places!

JA: Shorter technical papers are welcome in Acta Cryst F.

RS: Short technical papers in Acta F is an excellent idea.

GM: Are they supported by CCP4? Most funding bodies now require (at least larger ones) and pay for this.

JA: Supported as in open access fee paid for by CCP4? I think it would have to be related to CCP4 SW?
 DR: Universities may have OA funds, and the hosting University often has a mechanism to provide funds – this would save CCP4 funds and help contents to get published that is not strictly related to the SW!
 MH: For a lot of Unis RCUK funded research is covered for OA but not if its funded from elsewhere
 GM: We could use biorxiv as an open repository. At least before the final version.
 TP: F1000 may be another possibility. <https://f1000research.com/>
 DR: F1000R is more a regular journal, just with review post-publication
 PM: I like the idea of reviving the CCP4 newsletter, but this needs an "editor"!
 NP: Are we not describing a blog? People could post less formal things there ...

The discussion will have to be continued and include a connection to CCP4 program documentation.

3. CCP4 activities, workshops and courses (Eugene Krissinel)

The biggest event, no doubt, is release of CCP4v7.1! However, there are other significant developments:

a. Cloud (Eugene Krissinel, Oleg Kovalevskiy)

CCP4 cloud now integrates user support for licenses by 3rd party license framework. This may be attractive for users, and also increases visibility by linking up with other packages

Selenium tests. Testing shall be integrated with integration of software. Procedures, integration, "smoke tests" to test overall functionality. Current 538 executables, Jenkins test for 281 of these (52%). For developing further tests on any software that does not yet have a test please contact Oleg.

Some programs do not have a test, often GUI dependent. This will require full switch to Qt5.

PyTest is a Python script that communicates to web browser via selenium. This can work remotely, and then serves the CCP4Cloud web-server.

KC: runtime?

OK: nightly build needs test. Longer tests, if required, must run weekly.

TB: Why not use this for testing Qt4 GUI? <https://doc.qt.io/archives/qt-4.8/qtest.html>

PE: Coot has a comprehensive test suite built in.

CB: We use the pytest framework for automatic tests. We wrap others

b. CCP4v7.1 (Charles Ballard)

CCP4v7.1 released in April: Cloud and Gemmi are significant advances, also migration to coot0.9. Update 001 is major, update 002 being tested. Migration to Python 3 and Qt5 are urgently needed, but this is a major body of work.

KC: Are Gemmi exposed interfaces still changing?

CB: yes, but the deposition is the important issue that needed resolving and demanded release.

c. Documentation (Eugene Krissinel, Maria Fando, Ivo Tews)

Derived from workshops, we realised that we need "user guidance". We can call these verdicts. Is this a development for AI potentially?

KV: users don't know what they do not know. Path' into documentation?

KC: expertise to verdict. Encoded in i2 already.

Developers do not necessarily document well / all features. Perhaps we should have an open project for this? Repository of documentation files would then happen via GitLab. But we need to make sure developers and programmers contribute. Documentation currently for 24 out of 35 tasks. Then branch to contents.

EK showed demonstration projects, this is a helpful feature for education! This received praise by all.

4. CCP4 activities, workshops, roadshows (Charles Ballard)

The following workshops and schools were planned:

- Madrid
- Rapiddata
- BCA summer school
- APS, Chicago, Jun 15-22
- SWSBC June
- IUCr, Aug
- Uruguay, Sept
- Spring-8, Japan, Oct start
- India, Oct/Nov?
- Shanghai, Oct?
- DLS Nov
- GRC (sponsor)

All this year are postponed (still to confirm Japan) or cancelled, bar DLS which will be virtual in December. Several organisers are not happy to go the virtual route.

- South American workshop is now Sept 2021
- APS June 2020
- Thailand - early 2021 depending
- South Africa - as soon as clear in.

5. Experience with online workshops and conferences (Ed Lowe, Tom Burnley, David Waterman)

Ed Lowe: Online taught course. Crystallography course, open to others. Practical parts are skipped. More online meant more students. Limiting session to two hours. Use MS-teams, keep chat channel open, and have a monitor person (moderator). Flipped learning (talks available before the presentation). A total of 50 participants was divided up into 10 people workshops with an individual instructor.

NP: Use Zoom breakout rooms?

DR: Can Cloud projects be shared?

DW: My understanding is yes, with the next or subsequent update. The technology is there, the problems will be more human things - engagement, understanding, fatigue...

AC: Can you use virtual machines? Did a workshop this way recently but did not share machine with supervisor?

ED: Maybe ask students to share data in advance, and then set up one-to-one hours to go over problems.

RK: Another problem is network connectivity. Infrastructure in places like Uruguay and South Africa is poor compared to Europe and links to Europe and North America are very slow.

DR: We would need to be confident that bandwidth was sufficient to avoid frustration/wasted time

KC: The installation problem is my experience too. We need to deal this proactively. Maybe have an installation session on the first evening with running a trivial job as the goal?

MV: make sure to give them a Linux tutorial as we used to do; can also include some basic IT background; virtual machines or CCP4 cloud for everyone then...

KC: Students often don't even understand folders, because search is so powerful.

SMN: We are not controlling what OS people use. There will likely be mix of Windows and Mac, with probably lower number of Linux. We have to cope with all 3.

DW: DLS online workshop. Rather intense format. Social events are very useful (find that also depends on success for the early events, posters and then towards the end presentations by the students). Messages for

this year's was to stop, but decision was taken then to run virtually. Intensity not working, so extend to 2 weeks in office hours. Bursaries given out for childcare.

GM: In many countries students do not ask questions until they know tutors.

RJ: It works better if tutors can be proactive and go to students who haven't asked questions yet.

MH: My experience in online meetings (non-ccp4) has been that students are more likely to ask written questions in a Zoom Q&A or chat than they are verbally

DR: Colleagues say students are *more* inclined to ask questions during online lectures than normal

AP: Experience from iNEXT-discovery kick-off meeting, normally three days: It was split to several events: A pre-recorded video for the background, a live session for all, a management meeting on a different day, and advisory board meetings on different days. There was no reason to keep all these on one day, they were split to two weeks, and a mix of (little) prerecording and live, saved time for everybody (eg our SAB watched the "background"video", the Pls did not.

JT: CCP-EM was greatly enjoyed by many people in York. We had a Discord page open to chat to each other during the lectures, which made it even more engaging.

KC: The cost benefit means a lot of people on the edges of the field, students, and ECRs can come to the meeting. Childcare also a huge benefit.

6. Experience from organising a CCP4SW (Jon Agirre)

Improvements to the networking event were discussed, such as:

- posters session (received no support)
- stickers for keywords of interest (endorsed)
- quiz (endorsed)
- food and drinks
- merger with speaker's dinner
- childcare

New in the program - extra time at the end of each session for questions (also as slack). However, presently the program ends after 5pm, however the venue needs to be vacated by then!

It was noted that the cost of drinks in the venue is (too) high for students. Therefore, would it be possible to get a sponsor for this event?

KC: The 'What's new' session doesn't usually go in the proceedings. Should contributors be given the option? (Or are they already?)

MH: I think a composite 'new developments' article in the proceeding is a great idea - including useful but 'small' items that could not make a full paper

7. CCP4 SW2021 "Integrating Structural Biology" (Atlanta Cook, Dan Rigden, Tassos Perrakis)

Combine from different sources to broaden your structural biology. Plan for a live online format. Structure:

Session 1 – Structural Bioinformatics 1 – pre structure analysis

Session 2 – refinement, best model (cray, neutron, EM image and diffraction)

Session 3 – dynamics (computation, ensemble, NMR)

Session 4 – interactions (ligands, fragments biophysics, single molecules)

Session 5 – chemistry (XFEL, caging, lasers, catalysis, spectroscopy, QM/MM)

Session 6 – Multi-methods modelling (MS/SAXS/cryoEM, validation)

Session 7 – In cell (cryo EM tomography, Xrays, NMR, single molecule)

Session 8 – Structural Bioinformatics 2 (post structure)

Online. But are the sessions too long? Or can we have a meeting spread over several days with a session per day? Votes for avoiding a weekend, extending the meeting to four days, and on having 2x2hrs session in each afternoon; afternoon timing to also cater for and maximise US participation.

TB: To increase 'new' speakers esp. early career you could consider inviting abstracts and selecting from those. At the CCP-EM symposium those talks were generally very good.

EK: Abstracts sound like a rather interesting idea, which we never tried before.

AP: Eight sessions, plus the "synchrotron meeting" and "What's New" beforehand will take a lot more time out of the start of the year.

JT: Some of it parallel, as it is recoded anyways?

ED: You realise your afternoon sessions go over school collection times!

DR: Parallel sessions is something that online allows more easily

ED: One important part of these meetings is forcing you to listen to new material - parallel sessions makes that harder

AP: I do not like parallel sessions. really not.

RF: No parallel sessions. Spreading out over afternoons sounds good. Worked nice for CCP-EM.

RK: It's worth noting that the SW2020 was broadcast through Zoom. There were about 120 viewers.

KV: I would recommend considering longer Q&A sessions: it takes much longer than a quick shout from the back and a quick answer by speaker. And without extensive Q&A sessions it would become again closer to a lecture series. Remember, there are no coffee-break talks for students to catch up with speakers.

MH: Other zoom conferences I have taken part in have some questions fielded verbally by the speaker, but those that there isn't time for are then answered in writing within the Q&A feature of Zoom afterwards.

NP: Using cahoot for pub quizzes works phenomenally as far as I have experienced.

8. New software

This section was postponed to the next WG2 meeting.

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

Proposed date: proposal 24th September 2020, online.

10. AOB

Is this format acceptable, comments? Should we plan to hold WG2 meeting online in future?