Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 29th September 2020	**Time:** 09:00 – 13.00
Location:	zoom	
Circulation:	ccp4wg2@stfc.ac.uk	
Attending:	Jon Agirre (JA), Charles Ballard (CB), Arnaud Basle (AB), Dave Briggs (DB), Atlanta Cook (AC), Eleanor Dodson (ED), Paul Emsley (PE), Stuart Eyres (SE), Vilmos Fulop (VL), Mike Hough (MH), Robbie Joosten (RJ), Ronan Keegan (RK), Eugene Krissinel (EK), Ed Lowe (EL), Stuart McNicholas (SMN), Mark Morgan (MM), Garib Murshudov (GM), Rob Nicholls (RN), Martin Noble (MN), Nicholas Pearce (NP), Anastassis Perrakis (TP), Dan Rigden (DR), Alan Roseman (AR), Pietro Roversi (PR), Ivo Tews (IT), Ville Uski (VU), David Waterman (DW), Keith Wilson (KSW)	

5 mins breaks at every full hour

09:00-13:00

1. Approval of minutes from July WG2 meeting
2. Chairs report (Ivo Tews)
3. CCP4 SW2020 Special Issue (Jon Agirre)
4. CCP4 SW2021 "Integrating Structural Biology" (Atlanta Cook, Dan Rigden, Anastassis Perrakis)
5. CCP4 SW2021Dates, format of the SW (Charles Ballard)
    a. CVent conferencing software (Stuart Eyres, Ronan Keegan)
    b. What's New, Lunchtime bytes (Ville Uski, Ronan Keegan)
    c. Dates and format (Charles Ballard)
6. New Software
    a. What's new in CCP4 (Eugene Krissinel)
    b. Refinement targets and scattering methods (Garib Murshudov)
    c. CCP4i2 (Martin Noble, Kyle Stevenson)
7. next meeting: 20th January
8. AOB

Minutes

1. **Approval of minutes from the online WG2 meeting 30/7/20 (Ivo Tews)**

The minutes from the online WG2 meeting 30/7/20 were approved online, following the meeting.

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

The new web pages based on WordPress are out, many thanks to all involved, in particular Ville Uski. WG2 had discussions / suggestions on how to add to the section for reporting problems and contacting CCP4.

Adding to the report from SWSBC2020, prizes have now been given out as published online, sponsored by CCP4 and BCA. There is also a note un the BCA proceedings on the successful online meeting.

The online format made various changes to the SW necessary, including one out-of-rota WG2 meeting, and there were and still are several additional meetings required to discuss the technical side.

3. **CCP4 SW2020 Special Issue (Jon Agirre)**

Jon went through the state of papers submitted, reviewed and accepted. There are still outstanding submissions, and there were some cancellations. “More challenging than anticipated”. The target is to publish by the next SW2021, and have a total of 18 contributions, roughly.

4. **CCP4 SW2021 “Integrating Structural Biology” (Atlanta Cook, Dan Rigden, Anastassis Perrakis)**

Discussions on speakers have continued since the last WG2 meeting, and a new list of speakers is presented, whilst 42 invitations are now out (but several require chasing). The online format in the afternoon caters for Europe, Africa, much of Asia and America. The approved structure of the meeting is as follows:

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)

Two bioinformatics sessions bracket this programme: the first is on characterising targets, the one at the end about analysis of the structures. Sessions then focus on the models generated, interactions, dynamics and finally integration of different methods. The penultimate session introduces structural biology in cells. Overall, this is a very broad programme. The first morning integrates CCP4 – What’s New, and LTB are on the other days just before the meeting starts. The social programme planned includes a quiz and games.

An online meeting gives two advantages, cutting out travel and asking speakers from further afar. Also, talks can and potentially be shorter to keep the attention span. What follows is that this then creates opportunity to invite more speakers. The WG2 group discussed the sessions in detail, and suggested speakers. Talks should be didactic, and there should be emphasis on good introductory talks.

The need to up the ante on social and framework program was discussed. While we cannot recreate a live event, best effort should be made to allow people to meet in online social and breakout rooms, to ask questions to the speakers and to socialise, which is part of the essential study week experience. We could also add interactive elements. Input needed.

GM: Games are fine, but can there be time for scientific discussions? Perhaps foster by popular scientific themes.

RJ: these are not mutually exclusive; you can have both; provide many rooms.

TP: Normally, there is nine-2-five sciences, but also five-2-midnight very important interactions, where you catch up with an old colleague, or you sit with someone for dinner, and this is an important component of a meeting. With breakout rooms it's usually a disaster, people do not join. Therefore, we need structured activities. Interactive polls are also useful.

IT: in any case, we will provide a software platform that will allow for all these things you plan. What is needed in all of this still is a moderator, and you need to incentivise participation.

AC: There will be opportunity for people who want to catch up. But we have to find a way for younger people to find their peers, and that is really difficult in an online format.

IT: Maybe there should be an option for participants to start their own rooms if something comes up, to get a more dynamic interaction going.

TP: To get people to participate, you could do sessions like "ask the expert", and even host these by a team. For the break between sessions there are questions but nothing else, and I may be a minority vote for saying: an hour of nothingness is a bit long, so there could also be activities in the break between sessions.

Several people remarked that the break should be completely free not to exhaust participants.

Plans for the special issue: There are three categories now, because of the large number of speakers and the resulting long list of articles that could emerge as a special issue. (1) required, if this is essential for the special issue, while the other two categories are (2) strongly encouraged or (3) encouraged for a special issue.

5. **Dates and formats for the SW (Charles Ballard)**

   a. **CEvent conferencing software (Stuart Eyres, Ronan Keegan)**

We have looked at a number of different software solutions that can provide online conferences. CEvent was looked at, and the Global Research Council's Conference are using it in November. This can serve as a test for CCP4. But there are other software solutions that are also attractive, one is Meeting MoJo. Each of these has their unique selling points, and the decision has to be made after all have been seen, followed by procurement.

Generally, participant numbers up to 10,000 are fine, and we can offer breakout rooms etc. A key requirement is the registration element, as this is a public meeting, and we need to be able to monitor and control attendance.

DR: it would be interesting for us to know what the sort of main selling point for CEvent is, compared to generic solutions like Zoom. This then might trigger other options in our mind.

SE: Zoom as an option, for example, is difficult because it is about managing the number of people and providing an experience for the user inside a navigation, not just to go to a website.

What will have to follow this WG2 meeting is a discussion on technical features the organisers would want to see, and then a selection of the best platform to provide this. This will then be discussed in detail with the software providers, before taking the final decision.

   b. **What's New, Lunchtime bytes (Ville Uski, Ronan Keegan)**

The first morning is reserved for the "What's New" session, planned 11-12:30 with the main meeting starting at 1 pm. Lunch Time Bytes on the other days, with six running in parallel. WG2 discussed whether timing was right, or whether there should also be an offering be made in the evenings, but consensus was morning

sessions, only. Scope for a "clinic" that we had with the Molecular Replacement meeting (bring your problem) was discussed but did not seem to be a good option for the topic of this Study Weekend.

c. **Dates and format (Charles Ballard)**

Registration later than normal, it overall running well for preparation for a SW online 5-8th January.

6. **New software**

a. **What's new in CCP4 (Eugene Krissinel)**

Updates since June are release and updates (Charles Ballard). Online services and web site are updated (Ville Uski), as well as adopting STFC cloud resources (Ville Uski, Ronan Keegan, Charles Ballard). New services include CONPLLOT from Liverpool. Activity also for CCP4 cloud, where now 200 cores at STFC are allocated and set up under a very convenient framework, and documentation - all is updated synchronously; CCP4-online is being migrated from CCP4 machines to STFC cloud (Eugene Krissinel, Andrey Lebedev, Maria Fando, Ville Uski). Further development is incremental in the absence of workshops and active feedback, as the focus is on debugging and tests. Tests are now running regularly (Oleg Kovalevskiy). There are also new video tutorials on for cloud, and a roadmap guiding the user through CCP4 cloud, contact Eugene if you want to publicise materials. We presently have 25,000 setups for CCP4v7.0 and CCP4v7.1 is now catching up.

b. **Refinement targets and scattering methods (Garib Murshudov)**

Sources that can be used now Xray data, EM data, NMR, Neutron; refine against AceDRG stereochemical knowledge (similar structure to ProSMART). NMR restraints need adding to refmac5. Novel approaches to integrate radiation damage for refinement are being developed. Garib discussed errors in data, description of electron diffraction / scattering, electron potential and hydrogen refinement (Nakane et al Nature. 2020 Nov;587(7832):152-156. doi: 10.1038/s41586-020-2829-0). Further data shown on Neutron diffraction refinement (Lucrezia Catapano) with modified library with specific proton distances for neutron/electron/Xray (Fei Long). We need clean experiments with X-ray/Neutron/ED – can two of them predict the third?

c. **CCP4i2 (Martin Noble, Kyle Stevenson)**

There are different users, looking at documentation at different levels: basics, Information not specific to a pipeline or GUI, specific documentation. Presently there is CCP4i2 documentation and CCP Cloud documentation with an overlap; much of the present is HTML. Presently, there is an online and an offline system for GUI2 that can get out of sync. CCP4Cloud uses markup language migrating over to rst (reStructuredText; while MD language would be an alternative; Twiki not an alternative as it does not produce proper PDF) with Sphinx to compile (pip install sphinx / sphinx-tabs / sphinx-rtd-theme, with pandoc to convert html to rst; continuous integration in Gitlab). An ideal case scenario is an easy system that can be added on by the user base, like a wiki, and new users may find this easy.

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

Proposed date: proposal 20th January 2021, online.

8. **AOB**

Rota of meetings was discussed, based on the new virtual meeting schedule. It was discussed we would have more meetings, and possibly separate business / core / study weekend organisation and then scientific meetings. These would not be replacing workshops. This will be trialled and taken forward for further evaluation.