



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 30 th July 2020	Time: 09:00 – 13.00
Location:	zoom	
Circulation:	ccp4wg2@stfc.ac.uk	

5 mins breaks at every full hour

09:00-13:00

1. Approval of minutes from June WG2 meeting
2. Chairs report (Ivo Tews)
3. CCP4 SW2021 “Integrating Structural Biology” (Atlanta Cook, Dan Rigden, Anastassis Perrakis)
4. Experience with online formats
 - a. Feedback from SWSBC (Ivo Tews)
 - b. Feedback from SWSBC/CCP4 Roadshow (Stuart Mc Nicholas, Ed Lowe)
5. Dates, format of the SW (Charles Ballard)
 - a. How to lunchtime-byte (Ville Uski, Ronan Keegan)
 - b. How to do the DLS satellite meeting (Ralf Flaig, Pierre Aller, David Waterman)
 - c. Open discussion on online formats (Ed, Ivo, Jon, Ronan, Ville, Randy, Atlanta, Dan, Anastasis)
6. New Software
 - a. progress on ED (Tarik Drevon)
 - b. Deposition of multi-method datasets (Sameer Valenkar, John Berrisford)
7. next meeting: 24th September
8. AOB

Minutes

1. Approval of minutes from the online WG2 meeting 29/6/20 (Ivo Tews)

The minutes from the online WG2 meeting 29/6/20 were approved online, following the meeting.

2. Chairs report (Ivo Tews)

There were some probing discussions in the background whether the **Northern Structural Biology Meeting** can be continued, as there would be support by the CCP4 available and there would be interest. The issue of location would not be a problem if this was an online format, such as SWSBC2020 (see below), however it was not possible to identify suitable candidates that would organise such an event this year so we need to look at organising this in 2021.

COVID19 has interrupted the usual rota of meetings and workshops. Many meetings were cancelled or postponed. The SWSBC2020 meeting took the decision to give a go-ahead for an online event advertised as a collaborative event between eight SWSBC consortium partners. The event included five scientific sessions, including Enzymes, Complexes, Biotechnology and EM as well as two plenaries on EM and XFEL science, a poster session, a social, and a CCP4 Roadshow.

The new web pages based on WordPress are out. They are easier to maintain by the core team, have feeds for news, meetings and positions, and are built from scratch. Please feed-back comments.

Ongoing discussions concern how we communicate, document and publish CCP4 activities. Two points from ongoing discussions: (1) we must make an effort to comment and document software from within, e.g. in the interface users see and use; (2) We are aware that there are ideas worth publicising and sharing, yet they will not be publishable as they cannot be accepted as scientific papers. We must follow up on these insights.

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

The draft programme was presented by Atlanta Cook and discussed in the WG2 group. The WG2 group discussed the sessions in detail, and suggested speakers.

4. Experience with online workshops and conferences (Ivo Tews)

a. SWSBC2020 (Ivo Tews)

The meeting was open (links shared on the web page) and had one point of contact for abstracts. After sorting into five topics, the remainder of the selecting talks and posters was decentralised and done by five different universities who chaired these sessions. This is a new democratic format for organising conferences, where the organisation is shared, and meetings are open.

The meeting additionally had two plenaries which were well received, a CCP4 roadshow (see below), and a poster session. Form 24 poster submissions, each poster presented in its own chat-room in screen format, which can be improved as there was not enough traffic in those channels. Ten posters were chosen for 2 ½ minute poster pitches, which was a very well received session.

We have had a plethora of feedback and comments that are very useful to understand better what is needed in an online conference. The main and recurrent point is that short talks worked, and concise sessions are good, but there was not enough breakout space. It is therefore clear from this experience that an extra effort needs to be made for online conferences for people to meet, aka. virtual coffee rooms.

b. CCP4 events: Roadshow at SWSBC2020 (Ed Lowe, Stuart McNicholas)

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.

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

a. How to lunchtime-byte (Ville Uski, Ronan Keegan)

b. How to do the DLS satellite meeting (Ralf Flaig, Pierre Aller, David Waterman)

c. Open discussion on online formats (Ed, Ivo, Jon, Ronan, Ville, Randy, Atlanta, Dan, Anastassis)

Plans for LTB, the DLS satellite meeting and on format of the meeting were discussed in the meeting. It was agreed to have further technical meetings offline, owing to the complexity of the issue.

6. New software

a. Progress on ED (Tarik Drevon)

b. Deposition of multi-method datasets (John Berrisford)

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

Proposed date: proposal 24th September 2020, online.

8. AOB

None.