



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 24 th January 2018	Time: 11:00 – 16.00
Location:	Birkbeck, University of London, Seminar room 612 (entry from Torrington Square)	
Circulation:	ccp4wg2@stfc.ac.uk	
Signed up:	Charles Ballard, Nora Cronin, Eleanor Dodson (ED), Mike Hough, Ronan Keegan, Eugen Krissinel (EK), Andrey Lebedev, Ed Lowe, Airlie McCoy (AM), Karen McIntyre (KMc), Rob Nicholls, Arwen Pearson, Randy Read, Dan Rigden (DR), Kushwant Sidhu, Kyle Stevenson, Ivo Tews (IT), Ville Uski	
Apologies:	Dave Brown, Vilmos Fulop, Marc Morgan, Antony Oliver, Johann Turkenburg, Melanie Vollmar, Keith Wilson, Pamela Williams	

11:00-16:00 WG2 agenda

11:00-16:00

1. Approval of minutes from the London The Crick WG2 meeting 4/10/17
2. Chairs report (Ivo Tews)
3. CCP4 activities, workshops and courses (Charles Ballard)
4. Digest of the CCP4 SW2018 “Multi-Crystal and Data Collection”, feedback (Ivo Tews, Charles Ballard)
5. Talks: Molecular Replacement – state of the art and future
 - a. What happened in MR since SW2013 on Molecular Replacement (Randy Read)
 - b. Models, model quality and covariance (Dan Rigden)
 - c. Ensembles (Randy Read)
 - d. Limits: small fragments, multi-protein complexes (Randy Read)
 - e. Pipelines and online services (Ronan Keegan)
6. Open discussion – what topics should be included in the MR Study Weekend 2019 programme?
7. Proposals for organisers of the 2019 SW “Molecular Replacement”

Lunch

8. Whats new in CCP4? (Eugene Krissinel)
9. CCP4-on the web (Eugene Krissinel, Ivo Tews)
 - a. The new CCP4 Webpage, demo and discussion
 - b. Delivery from CCP4 Grant 2014: online services and interface
10. Hands-on (bring your own data): jsCoFE online interface for CCP4 (Eugene Krissinel)
11. Take note of the date of the next meeting (proposal 6th or 13th June 2018)
12. AOB

Minutes

1. Approval of minutes from the London WG2 meeting 4/10/17

The minutes from the London WG2 meeting 4/10/17 were approved.

2. Chairs report (Ivo Tews)

IT reported on presentations for WG2 at CCP4-Exec and to the WG1 during the SW2018. The “Pathway to Impact” for WG2 activities as part of the upcoming grant proposal was discussed; the layout of the new CCP4 webpages was proposed and shown. At the WG1, the SW2019 – Molecular replacement was confirmed.

WG2 then discussed how we can make WG1 more attractive and get people to contribute to this group. While the timing of the WG1 meeting clashes with “What’s New in CCP4” session at SW, it would be difficult to move this. There is a WG1 mailing list but its hardly used. Also, there is CCP4BB so why should people join? However, we could advertise for WG1 on the CCP4BB. KMc will invites UK commercials when they take out licence. Any further ideas? Would you please mail IT or Dave Brown.

Further, WG2 made a pledge for keeping the “Northern Protein Workshop” alive. With 35 attending the last meeting, better promotion through PIs in he North is urgent. CCP4-Exec is willing to support this meeting in future, or indeed welcomes further UK initiatives.

Q: How do we reach people who would be interested, through the CCP4BB and other means; perhaps requires an updated list of PI’s.

Q: Change the Carlisle location – Newcastle or Lancaster were suggested.

Q: Request from some students to couple CCP4-North with a CCP4 workshop might be an opportunity.

IT reported that 2019 is the “40 years of CCP4” anniversary. There is a central meeting to be held in London, possibly at Royal Society. Would CCP4WG2 have ideas support this further?

Q: Amend the SW2019 – Taking over “What’s New” section with some historic notes > “What’s OLD?”

Q: Getting a CCP4 40th Anniversary memory stick with all SW proceeding:

A: This would need to negotiate with IUCr for ActaD ones but is possible

EL: Can put teaching tutorials on the stick, this would require 8 GB; this is Linux which may not boot on MACs

Q: Put links on stick to websites, documentation and tutorials.

IT suggested to shift the WG2 meeting start time to 11:30 (rather than 11:00) to allow people more time for travel and purchase of OffPeak fares. Agreed.

3. CCP4 Core Group Activities (Charles Ballard)

The activities in workshops and supported course have averaged as 1½ per month in 2017. The burden to run these is two to five core team members per workshop, two for a conference. Discussion on who can help: More helpers would be good, core team is usually asked first; however it would be good to have a “one stop shop” where people can take someone through the whole process; these might be users very familiar with CCP4 with plenty of data processing experience. It would always be desirable to have local people assisting. Help is mainly needed for working with data, not so much with the tutorials.

The following were supported:

- January: CCP4 Study Weekend (UK) – conference organisers
- February: CCP4/SPring-8 workshop (Japan) – workshop organisers
- March: Oulu (Finland) – workshop tutors
- April: RapiData (USA) – workshop tutors/sponsors
- May: 1) Macromolecular Crystallographic School (Spain) – workshop tutors/sponsors
2) ACA (US) – conference attendees
- June APS/CCP4 school (USA) – workshop incl. data collection organisers
- July SWSBC meeting (UK) – conference sponsors/demonstration
- August 1) IUCr 2017 (India) – conference attendees with workshop/demonstration
2) IUCr computing school (India)– workshop sponsors
- September 1) BCA Summer School (UK) – workshop tutors/sponsors
2) Northern Crystallographic Meeting (UK)– conference tutors/sponsors
3) 3D electron crystallography (Switzerland) – conference tutors/sponsors
- October CAS/CCP4 school (China) – workshop organisers
- November Macromolecular Crystallography School (Uruguay) – workshop organisers
- December 1) DLS workshop (UK) – workshop incl. data collection organisers
2) CIUK (UK) – conference attendees
- On-going: DLS BAG training (UK)

Plans for 2018 include: **Definite** Jan: Study Weekend (conference); Feb: Israel (workshop); June: APS (workshop with data collection); June: SWSBC (conference); July: ACA (conference); Aug: ECM (conference), ECM computing school (conference); Sept: BCA Summer School (workshop); Brazil (workshop); Dec: DLS (workshop with data collection). **Probable** Spring: RapiDate (workshop); Oulu (workshop); Madrid (workshop); Summer: Erice (conference); Sept: Northern meeting (conference); late 18 India (workshop); late 18 / early 19: SPring-8 (workshop with data collection). **Possible** Malaysia/Singapore (workshop); December; AsCA (conference); Request for joint workshop with Chinese Crystallographic Association in Beijing

4. Digest CCP4 SW2018 “Multi-Crystal and Data Collection” (Ivo Tews, Charles Ballard)

WG2 congratulates the scientific organisers Arwen Pearson, Max Nano and Robin Owen for a truly interesting and well organized meeting. The feedback has been overwhelmingly positive. Both, the scientific programme and the lunch-time bytes received positive comments, and comments were particularly good with students. The timing, not to hold the “study weekend” on a weekend, was also well received. Many problems from previous years seemed to not have occurred (e.g. timing, lunchtime bytes, queuing, rooms) as is clear from feedback. Our new network event received some mixed comments, and while it was generally very welcomed, we may want to start this a little later to give attendees a better chance to mix with people from the speakers dinner afterwards.

5. Talks: Molecular Replacement – state of the art and future

- a. **What happened in MR since SW2013 on Molecular Replacement (Randy Read)**
- b. **Models, model quality and covariance (Dan Rigden)**
- c. **Ensembles (Randy Read)**
- d. **Limits: small fragments, multi-protein complexes (Randy Read)**
- e. **Pipelines and online services (Ronan Keegan)**

6. Open discussion – what topics should be included in the MR Study Weekend 2019 programme?

WG2 discussed whether a session on EM should be included, either as a timely subject or as part of MR. Structural Biology is using EM as a tool, and there is the potential for cross fertilization of ideas.

WG2 also discussed whether we should include a session on Low Resolution. This also relates to EM as most LR are helped by EM.

Some topics of MR were discussed in more depth, for example how to Improve on a solution, and how to detect that there are not enough good solutions in order to come to a quicker exit from MR to engage in phasing strategies.

WG2 discussed that we should include real-life scenarios and practical talks of case studies.

Publication of the study weekend in the Conference Proceedings was discussed. The organisers were asked to communicate firm deadlines to the speakers.

7. Proposals for organisers of the 2019 SW “Molecular Replacement”

This part is not minuted. IT to approach potential WG2 suggested organisers after this meeting.

8. Whats new in CCP4? (Eugene Krissinel)

The Dials Gui “DUI” is now coming and ready for release by the time of the developers meeting before Easter. Auspex will be ready for release soon. The CCP4i2 development branch is to be released, and a consolidated update is to be released.

ED queried about mmcif dictionary; EK reported that this part is not ready yet.

9. CCP4-on the web (Eugene Krissinel, Ivo Tews)

IT presented a video demo of the new web page design. Remarks on CCP4 branding (AM), contact information (ED), Organisation of documentation (EK), and edit rights (DR); taken note of these comments. Next presentation of the web page design at the developers meeting before Easter.

10. Hands-on (bring your own data): jsCoFE online interface for CCP4 (Eugene Krissinel)

Live demo.

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

Possible date 6.6. or 12.6.2018, Location: London.

12. AOB

None.