Agenda

Meeting title:	CCP4 Working Group 2 meeting
Date:	Wednesday 21th September 2016 **Time:** 11:00 – 16.00
Location:	Birkbeck, University of London, Geology room 539 (entry from Torrington Square)
Circulation:	ccp4wg2@stfc.ac.uk
Present:	Charles Ballard (CB), Arnaud Basle (AB), Kevin Cowtan (KC), Nora Cronin (NC), Dave Brown (DB), Gwyndaf Evans (GE), Phil Evans (PRE), Mike Hough (MH), Ronan Keegan (RK), Nick Keep (NK), Eugene Krissinel (EK), Ed Lowe (EL), Airlie McCoy (AMC), Karen McIntyre (KM), Garib Murshudov (GM), Stuart McNicholas (SMN), Arwen Pearson (AP), Paul Rowland (PR), Kushwant Sidhu (SID), Ivo Tews (ITE), Ville Uski (VU), Melanie Vollmar (MV), David Waterman (DW), Pamela Williams (PW), Keith Wilson (KSW), Marcin Wojdyr (MW)

Please arrive for coffee at 10:30.
Directions http://www.bbk.ac.uk/geology/contact-us/how-to-find-us

11:00-13:00 WG2 agenda (only WG2 members)

1. Approval of minutes from the London WG2 meeting 8/6/16
2. Chairs report (Ivo Tews)
3. Acta Cryst Proceedings Issue "Protein-Ligand Complexes" (Paul Emsley, Judit Debreczeni)
4. Core group activities, CCP4 meetings and workshops (Eugene Krissinel, Charles Ballard, Kushwant Sidhu, Arnaud Basle, Ivo Tews)
5. Planning of the CCP4 SW2017 "From Crystals to Structure" (Keith Wilson, Mike Hough)
    a. Invited speakers and draft programme
    b. Plans for the Acta Cryst Proceedings Issue "From Crystals to Structure"
    c. Organisation of the meeting, Lunch-time-bytes (Charles Ballard, Ville Uski)
6. Ronan Keegan "SIMBAD - sequence-less molecular replacement" (Ronan Keegan)
7. Take note of the date of the next meeting (proposal 18. January 2017)
8. AOB

Lunch

13:30 -16:00 DIALS hands-on workshop (WG2 members and signed-up users)

9. DIALS - New software for diffraction image integration - an overview (David Waterman)
10. Results from DIALS for synchrotron data processing (Melanie Vollmar)
11. Latest developments in DIALS (James Parkhurst)
12. xia2/dials for ccp4i2 (David Waterman)
13. Practical part (see notes overleaf)
    a. Demo with the DIALS tutorial supplied in the distribution
    b. Hands-on help for participants - bring your own data
14. Feedback from participants

Minutes

1. **Approval of minutes from the London WG2 meeting 8/6/16**

The minutes from the London WG2 meeting 8/6/16 were approved.

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

Membership: the numbers of WG2 members on the mailing list are now at approximately 65; many of these attend the WG2 meeting, and are specially committed to WG2 issues.

There is second form of contacting a wider user base now, using direct mail to committed DLS bag contacts. Circulations through this route would invite for workshops and software trials, concurrent with the WG2 meetings. This happens – at the current rate – twice per year. Direct contact is dependent on volunteering recipients and their will to re-distribute information amongst members of their bags. The current list of contacts is (necessarily) incomplete, and I am happy to be contacted and to include further contacts.

Accordingly, the structure of the WG2 meetings has now changed. The mornings will deal with WG2 core business and be restricted to WG2 membership, while a practical part follows in the afternoon that should be open to the crystallographic community (by registration). We welcome user participation to receive feedback.

3. **Acta Cryst Proceedings Issue "Protein-Ligand Complexes" (Paul Emsley, Charles Ballard)**

We expect 20 articles for the special issue (out of 23); there are currently three articles accepted, seven are with authors for revision, one is with the referees, nine papers have not been received with the submission portal due to close end of September. Paul Emsley to phone to chase.

There was a discussion whether the PDB should be included in this issue, and whether a ligands specific CCP4i2 contribution should be included. Dave Brown agreed to speak to Stuart McNicholas, Sameer Velankar @ PDBe and Greg Warren.

4. **What's new, Conferences and workshops (Eugene Krissinel and Charles Ballard)**

CB reported on planning of meetings: ACA 22-26.7.16, BSR 21-24.8.16, ECM 28.8-1.9.16, CCP4SW 8-10.1.17, ACA 2017. IUCr 2017. CCP4 had a stand at ACA and IUCr but this option was not viable for the ECM meeting due to cost.

CB reported on planning and attendance of workshops: CCP4-APS Argonne, 21-29.6.16, 20 students; BCA/CCP4 Summer School, DLS, 21-26.8.2016, 40 students; DLS-CCP4, DLS, Dec-2016, 20 students; CCP4, Spring8, Japan, 23-27.1.2017, 20 students; CCP4/Institute Pasteur South American School, Montevideo, Uruguay, May-2017, 20 students

AMC reported on the BCA meeting, where we have seen a two-fold oversubscription in terms of applications to spaces – which meant had reserve list. All very good students and all engaged. The programme covered from applications to practical aspects, but it was clear that more focus should be on the basics of crystallography.

CB reported on planning of CCP4 sponsored conferences: rapidata, Standford, USA, 24-29.4.2016; SWSBC, Portsmouth, 27-28.6.2016, approx. 100 attendees; Northern Protein, Carlisle, 7-8.9.2016, approx. 35 attendees.

ITE reported on a 1 hrs lunchtime session by CCP4 / Jon Agirre at the SWSBC, attended by 25. This demonstration was warmly received and a good promotion for the use of Gui2, and discussion with users. This is generally better value for money than a stand at a conference.

AB/SID reported on the Northern Protein workshop, detailing programme structure and attendance. The programme included a two hour Workshop on CCP4MG. Here, too, the feedback from students was to deliver some fundamentals. Overall, the feeling was that more students at this meeting would be beneficial, and hence the ply for PI's to support students to attend these meetings.

After the discussion of the success of the Northern and South-Western meetings the question was raised whether there is room for a Southern / South-Eastern version which CCP4 might be able to support?

KC reported on a MOOC (Massive Online Open Course) for crystallography and suggested to look at education in one of the next WG2 meetings; this was met with consent. The suggestion was made to explore funding for a MOOC or to include in this as a proposal in the next grant application. The discussion included comments on bundling notes and videos and other teaching materials we already have, using a web repository, e.g. the BCA teaching materials that are already in a drop-box (AMC).

5. Planning of the CCP4 SW2016 "From Crystals to Structure" (Keith Wilson, Mike Hough)

The SW2017 will focus on ccp4 programs. Keith and Mike presented the proposed programme and speakers. The programme includes (1) Data Collection (2) Molecular Replacement (3) Experimental Phasing (4) Model Building (5) Validation and (6) Ligands recap and follow up; this was discussed in detail.

Some discussion about some of the talks in sessions 2 and 3 not being in the right category, and a suggestion that Experimental Phasing might best precede Molecular Replacement.

ITE criticised the gender balance of speakers.

The suggestion was made that for the CCP4i2 paper there should be a dedicated talk, e.g. a wrapping up talk by Liz Potterton.

ITE suggested inclusion of a Phenix talk – don't be afraid of the competion.

The suggested topic for SW2018 is "Multi Crystal and Data Processing" (unanimous) – DB/ITE to propose this to WG1 meeting at the SW2017.

6. SIMBAD – Sequence-less MR (Ronan Keegan)

In an exercise, Ample and Arcimboldo were used to solve some unsolved 14 year old data; a script was written to run through the entire PDB, using Phaser / Molrep, SHELXe, ArpWarp model building. The run took a 100 core processor 20 hours to solve. The result was an unexpected structure, which turned out to be a contaminant. *N.B. In the various CCP4 schools, we always get 2 or 3 cases of unsolved data due to contaminants or mistaken ID.*

This defines the goal: Rapidly test datasets using MR against PDB to identify known regular contaminants or novel contaminants, mistaken ID's, but also novel structures with structurally similar models in PDB. A ten-fold gain in speed is predicted in the use of AMORE and MORDA databases – in the above case 2 hours using a 100 core cluster. The top 200 scorers are put through full MR. SIMBAD available through CCP4 Online and

eventually CCP4 Cloud and now looking for testers – Contact Ronan and he will connect you to cluster as it requires a login.

7. **AOB**

The suggestion was made that on of the next WG2 meetings we might ask Jon Agirre to do a Privateer demonstration / workshop.

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

Possible date 18.1.2017, Location: London or DLS. Google poll to agree on date and location to follow.