Agenda

Meeting title:	CCP4 Working Group 2 meeting
Date:	Thursday 27th September 2018 **Time:** 11:30 – 16.00
Location:	Birkbeck, Philosophy, 30 Russel Square, London
Circulation:	ccp4wg2@stfc.ac.uk
Signed up:	Jon Agirre, Ben Bax, John Berrisford (JB), Dave Briggs, Dave Brown (DB), Eleanor Dodson (ED), Paul Emsley (PE), Carmelo Giacovazzo (CG), Luis Fuentes-Montero (LFM), Ronan Keegan, Nick Keep, Eugene Krissinel, Tobias Koryer (TK), Ed Lowe, Andrew Lebedev, Karen McIntyre, Marc Morgan, Garib Murshudov (GM), Rob Nicholls, Martin Noble (MN), Tony Oliver, Andrew Purkiss (AP), Dan Rigden, Mark Roe, Paul Rowland, Kyle Stevenson, Roberto Steiner, Melanie Vollmar, David Waterman (DW)
Apologies:	Charles Ballard, Kevin Cowtan, Mike Hough, Ivo Tews (IT), Isabel Usón

Please arrive for coffee at 11:00. **We will start 11:30** and break for lunch 12:30.
Directions http://www.bbk.ac.uk/philosophy/contact-us

1. Approval of minutes from the London WG2 meeting 6/6/18 (Dave Brown)
2. Chairs report, report on submitted BBSRC grant, CCP4 "pipielines" (Dave Brown)
3. CCP4 activities, workshops and courses (Ronan Keegan)
4. CCP4 SW2018 "Multi-Crystal and Data Collection", proceedings (Dave Brown)
5. Programme for the SW2019 "Molecular Replacement", Lunchtime Bytes, MR clinic, 40 years of CCP4 (Ronan Keegan, Dave Brown)
6. What's new in CCP4 (Eugene Krissinel)
7. Software – new developments
    a. jsCoffee – from data to deposition (Eugene Krissinel) (10+5 mins)
    b. SIR2018 – Molecular replacement (Carmelo Giacovazzo) (40+20 mins)
        i. The ingredients of the MR pipeline
        ii. The SAD –MAD techniques
        iii. Phase refinement process
        iv. CAT (evolution of Buccaneer)
    c. DIALS (15+5 mins)
        i. use of the new DUI (Luis Fuentes-Montero)
        ii. integration/scaling and other news (David Waterman)
    d. Refinement Validation (each talk 10+5 mins)
        i. Sheetbend molecular morphing; shift refinement (Eleanor Dodson)
        ii. ACEDRG Link Generation and new library (Garib Murshudov, Rob Nicholls)
        i. Accelerated deposition of multi-crystal PanDDA experiments (Tobias Krojer)
        ii. Molprobity integration into i2 (Jon Agirre)
8. Web Page Launch (Dave Brown, Karen McIntyre)
9. Take note of the date of the next meeting (proposal 23rd January 2019
10. AOB

Minutes

1. **Approval of minutes from the London WG2 meeting 6/6/18 (Dave Brown)**

The minutes from the London WG2 meeting will be submitted for approval in the January meeting (action IT).

2. **Chairs report (Dave Brown)**

DB reported on submission of the CCP4 grant proposal to the BBSRC and the review comments that were received (excellent). The proposal structure into four work packages was shown in the WG2 meeting in June. The focus of the proposal is on novel science and coverage of CCP4 to a large community, covering from expert to non-expert.

DB reported on design of CCP4 pipelines (topic raised in last WG2 meeting in June). This was dfiscussed in CCP4EXEC and should be a separate meeting to discuss this topic.

3. **CCP4 Core Group Activities (Eugene Krissinel)**

The following workshops and schools were supported or are planned:

- May: Madrid (Spain) – workshop
- June APS/CCP4 school (USA) – workshop incl. data collection organisers
- July: SWSBC meeting (UK) – conference sponsors/demonstration
- July: ACA 2018 (Toronto) – conference attendees with workshop/demonstration
- August: ECM Oviedo (Spain) – conference attendees with workshop/demonstration
- August: ECM computing school – workshop sponsors
- September: BCA Summer School (UK) – workshop tutors/sponsors
- October: Spring8 (Japan) – workshop
- October: India – SCIR, Chandigarh Workshop
- December DLS workshop (UK) – workshop incl. data collection organisers
- December: AsCA conference New Zealand
- New workshop in Thailand beginning of 2019

GM suggested there should be CCP4 representation at Gordons Conference on diffraction each year in future. DR said we could also plan to do this when abroad.

4. **CCP4 SW2018 "Multi-Crystal and Data Collection", proceedings (Dave Brown)**

Since there were non-responders to this issue, it is even more important to ensure that if speakers accept an invitation to talk at a study weekend, they must concede and know they are committed to deliver a manuscript.

5. **Programme for the SW2019 "Molecular Replacement", Lunchtime Bytes, MR clinic, 40 years of CCP4 (Ronan Keegan, Dave Brown)**

RK reported that the organisers had emphasized the need to contribute a manuscript when inviting speakers. They had good success with the invitations, as nearly everyone who was on the original proposed proragmme also accepted the invitation. The Study Weekend is now open for registration – link is on the CCP4 website.

RK reported on the *MR Clinic* which will be held on Day 1 as a Lunchtime Byte. Examples are from submissions and will be selected by the organisers prior to the SW. The Clinic will discuss selected problems and the solutions (if) found. The Lunchtime Bytes will be a maximum of 12 non-MR sessions.

DB reported on plans for the 40-years CCP4. There is the idea of including an informal presentation after the conference dinner. We might want to show how CCP4 has evolved over the years. A fun-thing to include would be a quiz at diner, screen shots of old GUIs, or how long it took running programs in the old days. There will be the 40-years CCP4 event at the Royal Society on 9th of July 2019 to lobby and highlight CCP4

6. What's new in CCP4 (Eugene Krissinel)

The CCP4 suite now includes Molprobity. The monomer library has been updated. The release bundles are repackaged automatically with every update. The "DUI" (Dials Gui) is now included and integrated with i2.

Planning is advanced for inclusion of SIR2018 (with new release). A developers release of the CCP4 cloud software is planned.

7. New software

a. jsCoffee – from data to deposition (Eugene Krissinel)
b. SIR2018 – Molecular replacement (Carmelo Giacovazzo)
    i. The ingredients of the MR pipeline
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c. DIALS
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EK presented jsCofE that has now been renamed CCP4 Cloud. New tasks include Image processing with Xia2 (images in client machine, results pushed to cloud temporarily). Also, using Coot for MR model preparation and general co-ordinate editing. Data preparation for deposition is actively being worked on, and a citation framework is being developed.

GM – PDB test report only created when start deposition test
DB – summarize which programs were successfully used
Action: EK – tag references with programme names
Developers will need to include a tracking mechanism.
Use of "same" monomer library will require agreement of the mmCIF Working Group.

CG presented SIR2018: Refinement of MR Phases, with several impressive examples. Functionality of enhanced *Buccaneer* building.

PE – question regarding licences/scripts/interface
CG: Licence - academic free, commercial – from CWR in Italy
PE – what happens next?
CG – more work on DNA RNA – Nautlius enhanced
GM – on paper/tables looks good, but should get test users
EK & RK agreed testing needed

LFM presented DUI (Dials GUI) improvements. Several new features are included:

- Zoom control on images
- Predictions and suggestions shown
- Bravis lattice explained
- Integration in CCP4i2
- DIALS image viewer integrated

AP – Box for refined parameters would be good
LFM – GITHUB issue tracker for problems or e-mail luis.fuentes-montero@diamond.ac.uk or dials-support@lists.sourceforge.net
DB – question and answers should go to CCP4bb – feedback has been good

DW presented news on the DIALS project. The Wellcome grant is coming to an end and a new grant is now needed / proposal in preparation. The main reference published: ActaD 2018 Feb 1;74(Pt 2):85-97. DOI: 10.1107/S2059798317017235. Also: serial crystallography signal improvement for XFEL paper out: ActaD 2018 Sep 1;74(Pt 9):877-894. DOI: 10.1107/S2059798318009191. New in DIALS are

- Dials.cosym – multi-crystal
- Dials.symmetry
- Dials.scale – scaling program

Scale into P1 first is recommended; no SG recommended – no systematic absences check yet
ED – reporting features are important
MN – XML file for i2 and .phil import
CG – electron diffraction still gives (too) high R-values
JB – Dials is 8th most popular in PDB; Xia2 (uses XDS/DIALS) has a problem in PDB deposition and does not report DIALS; DIALS should get better credit.

ED presented Shift Field Refinement. The procedure is best used post MR.

RN – how does it compare to model morphing?
ED – no report available yet – needs to be run in combination with Refmac to get statistics

RN and GM presented news on covalent link generation in ACEDRG and the new ACEDRG generated momomer library, updated from CCD.

TK presented accelerated deposition in XChem and PanDDA the "Event map". There is now an automated mmCIF format XChemExplorer and group depositions into the PDB are supported.

DB asked to clarify the correlation between event maps and fofc maps.

JA presented on molprobity integration in i2 and functionality to analyse geometry

GM – changes introduced in coot are not updated and require to run Molprobity again
PE – coot could perhaps display grey sticks for old model
DB raised concerns for the information generated on ligands

8. Web Page Launch (Dave Brown, Karen McIntyre)

KM showed the new CCP4 website www2.ccp4.ac.uk, which is still a work in progress. Comments that the font size on the mobile version was not right and that the buttons were too big. The aim is to get these web pages ready after the SW2019.

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

Proposed date: 23rd January 2019. Location: London.

10. AOB

None.