Agenda

Meeting title:	CCP4 Working Group 2 meeting
Date:	Wednesday 23th January 2019 **Time:** 11:30 – 16.00
Location:	Birkbeck, University of London, Seminar room 613 (entry from Torrington Square)
Circulation:	ccp4wg2@stfc.ac.uk
Signed up:	Jon Agirre, Svetlana Antonyuk, Charles Ballard, Arnaud Basle, Ben Bax, James Beilsten-Edmands, Tristan Croll, Dave Briggs, Dave Brown, Luis Fuentes-Montero, Kaushik Hatti, Nick Keep, Ed Lowe, Airlie McCoy, Karen McIntyre, Stuart McNicholas, Marc Morgan, Kamel El Omari, Nikos Pinotsis, Andrew Purkiss, Dan Rigden, Mark Roe, Pietro Roversi, Paul Rowland, Massimo Sammito, Kyle Stevenson, Ivo Tews, Ville Uski, Rangana Warshamanage, Pamela Williams, Keith Wilson, Martyn Winn
Apologies:	Ivan Campeotto, Kevin Cowtan, Mike Hough, Ronan Keegan, Eugen Krissinel, Rob Nicholls, Randy Read, Garib Murshudov, Antony Oliver, Isabel Uson, Melanie Vollmar, David Waterman

Please arrive for coffee at 11:00; we will start 11:30 and break for lunch at 1:30 pm
Directions http://www.bbk.ac.uk/geology/contact-us/how-to-find-us

11:30-16:00

1. Approval of minutes from the London WG2 meetings 6/6/18 and 27/09/18
2. Chairs report (Ivo Tews)
3. CCP4 Webpages (Ville Uski, Ivo Tews)
4. CCP4 activities, workshops and courses (Charles Ballard)
5. CCP4 SW2018 proceedings (Charles Ballard)
6. Digest of the CCP4 SW2019 "Molecular Replacement", feedback, attendance, dates for the study weekend (Ivo Tews, Charles Ballard, Dave Brown)

7. Scientific talks:
    a. DIALS scaling and updates (James Beilstein)
    b. Model tracing into phased density (Kamel El Omari)
    c. Model Quality: Privateer, molprobity, Edstats, prosmart_refmac (Jon Agirre)
    d. RIDL – quantifying radiation damage (Ed Lowe)
8. The CCPs – an overview (Dave Brown)
9. CCPEM session (chair Martyn Winn)
    a. Overview of CCP-EM (Martyn Winn)
    b. EM work at the MRC-LMB (Rangana Warshamanage)
    c. Lower resolution model fitting methods (tbc)
10. Open discussion – Study Weekend 2020 "Model Building", proposal for organisers
11. Take note of the date of the next meeting (proposal 29th May 2019)
12. AOB

Minutes

1. **Approval of minutes from the London London WG2 meetings 6/6/18 and 27/09/18 (Ivo Tews)**

The minutes from the London WG2 meeting were approved.

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

IT and CCP4 core are looking at pathways of software into suite, and guidelines are to be published on the web pages (core).

The issue of pipelines was discussed as an Exec agenda item

IT voiced an impression that the user base for CCP4 may be changing. Less groups focused on methods but wider life sciences base who might use CCP4 occasionally. This point was brought up for discussion at the last WG1 meeting.

The potential SW2020 topic was also discussed in WG1. There are about five topics that flow logically, and model building was due to be next. In the discussion, the topics low resolution, EM and validation came up. This is now for WG2 to decide on.

CCP4 roadshows were suggested at the CCP4 Exec meeting. However, this will need new volunteers in order to do these, and the topic is open, please respond to ITE.

3. **CCP4 Web pages (Ville Uski, Ivo Tews)**

The WordPress design is simpler and also more simplistic than the current website. It would be still possible at this stage to change the theme.

Some people that were testing had problems in connecting. VU demo-ed on screen, which solves the problem. In case of persisting problems contact IT, VU and KMc.

The STFC / UKRI logo needs to be at bottom of the screen, and funders need to be appropriately acknowledged before going live.

Additional background work is required: e.g. https certificates, but release by CCP4@40 in July is possible while transferring only relevant / essential contents (i.e. quick fix by covering from legacy site).

Documentation- link to other developers websites which they keep up to date. KW as long as relates to current documentation.

Contributing to the site: WordPress, written by Andy Collins (STFC Media), editors VU, KMc and IT.

4. CCP4 activities and workshops (Charles Ballard)

CCP4 roadshow - if want short 1-day introductory course at your institution contact EK / KW who are collating interest. Design first half of year and then run out. Road tested at AsCA meeting in Dec 2018 and went well. The Crick Institute registered interest (AP).

- New workshop in Thailand beginning of 2019
- June APS/CCP4 school (USA) – workshop incl. data collection organisers
- July: SWSBC meeting in Reading (UK) – conference sponsors/demonstration
- August: ECM Vienna (Austria) – conference attendees with workshop/demonstration
- September: BCA Summer School St Andrews (UK) – workshop tutors/sponsors
- September: Hamburg (Germany) – workshop
- September: Shanghai – workshop
- November: Uruguay, Workshop Organisers
- December DLS workshop (UK) – workshop incl. data collection organisers

The core team go to most workshops with developers, however there is scope to join these activities to help.

Query - is the strategy to reach out to communities where momentum is building up? We are present in South America but should also consider Africa. David Blow bursaries for Africa, India and South America are in place to come to the UK. Many people are consider the Pasteur for funding.

The APS workshop has had to start charging a few years ago, but this currently is not affecting applications for workshops. The DLS workshop was first undersubscribed due to lack of advertising, but finally was oversubscribed when advertised through WG1. We need to ensure to get publicity for activities such as the workshops offered.

Query – we have many citations from the APS workshop, this should become common practice.

CCP4 Release preparation early stage work on v7.1. Main feature include C++11 support (conversions in the background to stop having to port). GEMINI ccp4cloud distribution (early pre-release possible), pdb-redo code that are required for Phaser TNG. These changes are Windows 10 compatible.

Cycle up to Python 2.7.15 and support libraries. Continued work on WhatCheck for pdb-redo. Initial work on Bari suite has started. Continued updates slow down 7.1 Oreo. Recent updates included ARP/wARP (65) phaser (64), DIALS (64, shelve 67). Next 68 contains aimless, mrbump, is bad, ample, dui (major overhaul), Korda, amongst others. 69 planned: Dials 1.12.x, crank2, ccp4i2. It is planned to delay some updates in order to speed up release of v7.1.

Python2 to Python3 migration, and move to python3 compat as well as Qt5.11.12 and Pyeside by end of year, which is consistent with CCTBX timetable. Pyton2to3 running on test, contact VU. Running QT4 and Qt5 alongside is not practical, as it is rather bulky.

Plan to change building scripts in similar format to CCPEM. DIALS test runs at the end of our runs. Looking at running pietest type build to improve testing.

There is now a process for developers to test how new software fits into the CCP4 environment.

5. CCP4 proceedings (Charles Ballard)

Proceedings coming on, 9 papers accepted, four papers are in 2nd revision; there will be 14/15 articles in total this year. Publication date is Feb 2019 but may have to move into March.

Talks are being changed to format where talks can be put on Youtube and there will be CCP4 YouTube channel, while Q&A will be taken off.

6. **Digest of the CCP4 SW2019 "Molecular Replacement", feedback, attendance, dates for the study weekend (Ivo Tews, Charles Ballard, Dave Brown)**

The study weekend 2019 was a great success, and WG2 thanks the organisers for an excellent meeting. It was felt that the meeting did overall deliver a good mix of talks.

Remarks that have been heard: Larger font on badges; Less theory on SW but more technical stuff on programs; introductory talks were missed after Elena's lecture, which highlights the importance of structuring the meeting in a didactic manner, and it would probably help to have introductory speakers w/o requirement to having to publish in the special issue; definitions for some terminology was missed, as the sessions covered a lot of ground; the focus should be more on teaching aspects and getting the basics covered first; the balance of basics and interesting novel science should be maintained; the lunch breaks were too long, and lunchtime-bytes should run on both days; suggestion to adjusts the What's New and add a 101 session here to get some introductory knowledge; PI's miss the What's New due to overlap with the WG1 meeting but are interested (short summary of What's new in WG1?); the new "style" talks were welcomed as a change, i.e. DeepMind and Jenni's MicoED talk; due diligence required from WG2 on speaker selections.

Further feedback from delegates with KMc.

Discussion on the date of the SW (which can't be changed before 2021 due to commitments already made); this discussion had no consensus, and arguments in favour of middle of the week were given (students prefer this) and the attendance may relate to the date, so it should not be too close to NY. It was further discussed that streaming may have cut the attendance of the meeting down. Also, must consider DLS runs should not overlap. Limiting the number of participants will allow other venues to competitively bid for the CCP4SW, to be discussed in EXEC. This year, we had 150 students registered (some additional students were registering too late to obtain bursaries) and the rest of the attendance was PostDocs / PI's.

7. **New software**

Dials update - James Beilston Evans

What's New: post integration scaling and symmetry analysis; Xia2 dials-full pipeline - uses Dials scaling and symmetry analysis instead of pointless/aimless; Xia2.multiplex; Speed improvements to scan varying refinement & spot reduction for large datasets; Updates/fixes for EIGER detectors, nexus file formats; XIa2 - user can now set resolution limits for integration - detector limits set as default; Python 2 to 3 compatibility; Speed and memory improvements in dials.scale in live dev branch;
Upcoming dials 2.0: target date end April; Why - fully announce release of post-integration processing; Toolchain improvements planned; remove data lock data structure generated at import; consistent file naming throughout pipeline; move to alternative file formats; implementation of unique experiment identifiers to support multidataset Workflows; MmCIf output format for wwPDB depositions
New DUI layout: now available with an expert CCP4 update

Model tracing into Phased density - Kamel El Omari

Reported on practical experience using software. Auto building with ShelxE at resolution better than 2 Å: ShelxE autotracing works very well even with poor maps; building was improved with privateer; use nautilus - unusual conformation/poor maps; final model obtained with cycles of building 1 or 2 nucleotides at a time; Phase improvement, helped by building with S assignment; sometimes altering the solvent content can improve the secondary structure assignment. They are trying to improve the maps not the model building.

Conclusions: Building relies on the quality of initial maps; building is improved by improving maps
Difficulties: Beta strands at low resolution, disulphide vs main chain; building combined with phase improvement is very powerful; this sets a challenge for SW talking about model building: How do we help the users??

Model Quality: Privateer, molprobity, Edstats. Pro-smart_refmac - Jon Agirre

Privateer: Tools for spotting errors; Model vs data; Omit mFo-DFc maps using model and original data; Real space correlation for each monosaccharide; Model: ring puckering and confirmation, anomericity, absolute stereochemistry, nomenclature checks; SNFG diagrams of glycosylation (SVG), easier to spot funky lineages; support for fixing errors; connects to other programs via scripts and dictionaries

Graphical interfaces: CCP4i2, CC4mg, Coot, CCPEM (coming soon)

How to validate and correct structure automatically with Privateer, Coot and Refmac5? At lower resolution, even a correct starting model can result in a higher-energy conformation after refinement. Jon demoed with each package. Remark: colours for good/bad results need adding; loading correct dictionary will become easier once fixed in i2; Jon also showed how others are using the packages especially Privateer - journal articles; showed EDSTATS and clipper_python tools for validation.

CCP4i2 has a new interface for MolProbity. It produces a nice report with Ramachandran plots and various statistics.

RIDL - Ed Lowe

RIDL, a new high-throughput tool for quantifying radiation damage. RIDL is available on the Garman research group Github page.

8. **Open discussion – Study Weekend 2020 "Model Building", proposal for organisers (Ivo Tews)**

Topics for the Study Weekend 2020 which will be on Model Building. KW commented that they should cover all aspects of model building, including the cryo-EM.

Candidates for organisers of the Study Weekend were also discussed, and many names were suggested. IT proposed that at least one of the organisers should be from the EM community, and this was supported by several people.

9. **CCPEM session (Martyn Winn).**

Martyn Winn gave an overview on the CCPEM. There are currently over 7000 structures in the PDB which were solved using cryo-EM. Of those, nearly 30 % reached high resolution (< 5 Å). CCP-EM gets funding from the Wellcome Trust. There is significant overlap between CCP4 and CCP-EM, as many of the used software tools are the same.

Rangana Warshamanage presented the EM work at the MRC-LMB. Two new tools, ProSHADE and EMDA are to be released soon.

Sony Malhotra discussed model fitting with low-resolution maps.

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

Proposed date: 30th May 2019. Location: London.

11. **AOB**

None.