Agenda

Meeting title:	CCP4 Working Group 2 meeting
Date:	Wednesday 4th October 2017 **Time:** 11:00 – 16.00
Location:	The Crick, London (entry from St Pancras Station)
Circulation:	ccp4wg2@stfc.ac.uk
Present:	Charles Ballard (CB), Arnaud Basle (AB), Nora Cronin (NC), Phil Evans (PE), Luis Fuentes-Montero (LFM), Eugene Krissinel (EK), Ed Lowe (EL), Karen McIntyre (KMI), Stuart McNicholas (SMN), Marc Morgan (MM), James Murray (JM), Garib Murshudov (GM), Max Nanao (MN), Rob Nicholls (RN), Robin Owen (RO), Andrew Purkiss (AP), Khushwant Sidhu (SID), Kyle Stevenson (KS), Ivo Tews (IT), Graeme Winter (GW), Marcin Wojdyr (MW)
Apologies:	Jon Agirre, Mike Hough, Ronan Keegan, Arwen Pearson, Melanie Vollmar, David Waterman, Keith Wilson

11:00-16:00 WG2 agenda

1. Approval of minutes from the DLS WG2 meeting 12/7/17
2. Chairs report (Ivo Tews)
3. CCP4 Core Group Activities (Eugene Krissinel)
4. CCP4 Workshops and Courses (Charles Ballard)
    a. workshops and courses
    b. Organisation of the SW2018 meeting and Lunch-time-bytes
5. CCP4 SW2017 special issue (Charles Ballard)
6. Planning of the CCP4 SW2018 "Multi-Crystal and Data Collection" (Robin Owen, Max Nanao)
    a. Proposed programme
    b. Invited speakers and chairs
    c. Plans for the Acta Cryst Proceedings Issue
    d. Open Discussion
7. Outreach and teaching (Ivo Tews, Ed Lowe)
8. RABDAM – News for radiation damage detection (Kathryn Shelley)
9. GA – a genetic algorithm for merging of multi-crystal data (Max Nanao)
10. Requirements and Possibilities for Multi-Crystal Refinement (Garib Murchodov)
11. DIALS & XIA2 – News, development, future directions (Graeme Winter)
12. DIALS GUI – Development and Demo (Luis Fuentes-Montero)

13. Take note of the date of the next meeting (proposal 24. January 2018)
14. AOB

Break for lunch during the meeting.

Minutes

1. **Approval of minutes from the London WG2 meeting 12/7/17**

The minutes from the DLS WG2 meeting 12/7/17 were approved with one amendment (DW/GW to update DIALS section).

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

IT reported on good progress of the preparations of the study weekend 2018 and also the SW2017 proceedings. The plans for new software (v7.1) are to include several new pieces of software. These include MolProbity, PDBRedo, Whatcheck, Auspex, and may include others such as DUI – The Dials Gui, Rabdam.

IT reported on progress with the CCP4 grant proposal (coordinated by DB/WG1 chair). The application is planned for the BBSRC April round. The structure of the proposal was worked out in EXEC meetings in July and September (Exec head KW). WG2 is to enter as a Pathway to Impact proposal. Everyting is to be presented to WG1 at the SW2018. Contact IT or DB for more detail and for proposals.

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

The CCP4 suite v.7.0 has had 45 updates rolled out in a regular biweekly continuous release model. It is planned to consolidate release before 2018 to make installation even easier. To date, there were over 18,000 downloads of release CCP4v7.0.

Release 7.1 is in early preparation stages, as some components are not ready. Qt5 is being trialled; C++ 2011 and Python nearing end of life.

For the delivery of WP0 of the CCP4-2014 grant, there is a pre-release of jsCofE, Demo as lunchtime byte at SW2018, demo and tutorial to follow in the WG2 January meeting, volunteer testers needed. The interface uses the HTTPS protocol and will be available on the DLS server.

4. **CCP4 activities, workshops and courses (Charles Ballard)**

The activities in workshops and supported course have averaged as 1½ per month in 2017. 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)

AB discussed the fate of the Northern Protein Workshop in Carlisle, which has happened for the 25th year. The meeting is challenged and may not continue, due to low attendance numbers. There was also a shift from a larger fraction of students to a lack of students this year (larger proportion of PostDocs). AB suggested that PIs could support the meeting by attending and by supporting students to go.

The India workshop is new, and it is as yet unclear whether it can be continued. Expressions of interest for further workshops came from Malaysia/Singapore and China. It was discussed that there is continued demand on "headline" speakers (like GM) but there is also demand on having more people help with presentations.

5. Acta Cryst Proceedings Issue "Crystal to Structure" (Mike Hough, Charles Ballard)

We are on track presently with submissions and publication. Of 23 talks, a total of 20 articles are expected, for a January / February release (rather than December 2017 and January 2018).

6. Planning of the CCP4 SW2018 "Multi-Crystal and Data Collection" (Robin Owen, Max Nanao)

RO and MN introduced the detailed programme of the 2018SW with speakers and sessions assigned. The organisers have designed a programme with introductory talks, technical talks, and practical approaches. WG2 approved this programme.

The planned lunchtime bytes were discussed. The proposed structure is 1 byte per room per day (after the experience that two bytes per session was not good). It was discussed whether DIALS should run as an intro on day1 and an advanced session on day2. WG2 suggested not showing anything that cannot be immediately used.

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

7. Outreach and Teaching (Ivo Tews, Ed Lowe)

IT summarised the state of documentation that falls into three categories:

1. User documentation

User Documentation *may* be up-to-date, but scattered and distributed *via* various different routes (online or in program help). We have not been issuing a CCP4 manual since 2006 (but received a user request). While CCP4 is open to distribution of a Manual, there is the difficulty of resourcing this. The CCP4 Wiki serves an important role in the absence of a new manual; clearly, the Wiki also needs attention (Kevin Cowtan needs support and help for this).

2. Developer documentation

Most of CCP4 developers are not directly employed by CCP4, so getting documentation in one format may be difficult and needs effort. However, since developers typically are interested to let the users know how their programs work and how they can be used, this part of documentation is typically up-to-date for new programs (less so for elder software).

3. Tutorials and lecture materials

There are many tutorials available through the CCP4 website. However it might be an advantage to produce a distribution. A disk (branded CCP4 stick) has the caveat that it immediately becomes obsolete. Instead, a designated portal/repository is suggested that can be updated, and has the advantage of having tutorials in a central place.

EL gave an introduction to crystallography using CCP4 on Linux. The tutorial includes chapters on Data Processing, Phasing and Model Building. To run this, Ed showed how everything (tutorials and software) is packaged on a single USB stick.

KS reported on documentation for CCP4i2. The material on the web pages includes tutorial examples and an introductory video by Kevin Cowtan (YouTube). Navigate to the new documentation via Projects → CCP4i2 or Documentation → CCP4i2. We now need a structure for keeping and growing the information. The suggestion is to migrate contents early to the new WordPress website.

Suggestion from GW to consider CCP4BB as the richest information source.

IT: will be linked into the new web pages.

8. RABDAM – News for radiation damage detection (Kathryn Shelley)

KS introduced RABDAM, a program developed in Elspeth Garman's group to identify specific radiation damage artefacts within individual protein crystal structures. The ability of RABDAM to detect known sites of specific damage within damaged datasets by calculating the BDamage metric (a derivative of atomic Bfactor corrected for packing density) was demonstrated. In addition, validation of the newly developed Bnet metric (a derivative of BDamage that summarises the extent of damage suffered by a structure in a single value) was presented, including evidence that the Bnet values of different structures can be fairly compared with one another. The potential use of RABDAM to assess the quality of structures deposited in the PDB from a radiation damage perspective via its calculation of Bnet was suggested.

Discussion points included the limitations of the BDamage metric, such as its lack of comparability between structures (resulting in an inability to provide a threshold value for damage analysis), and its dependence upon structure refinement quality. Several useful suggestions for improvement of the code were also made, for example the possibility of increasing the speed of the packing density calculation by accounting for the position of the asymmetric unit within the unit cell. The *cif format was suggested to report resulst and output, to avoid overwriting the B-column of the PDB file.

9. GA – a genetic algorithm for merging of multi-crystal data (Max Nanao)

MN presented our study of merging synchrotron serial crystallographic data. A frequently encountered problem is that of non-isomorphism between crystals. We using a genetic algorithm that uses merging statistics for its target function in order to select which datasets to merge. This method, in the test cases that we examined, produced results that met and in some cases surpassed the current HCA based methods. The method was recently published (https://www.ncbi.nlm.nih.gov/pubmed/27599735) and a python script demonstrating the concept is available here https://sites.google.com/site/codgas1/.

10. Requirements and Possibilities for Multi-Crystal Refinement (Garib Murchodov)

The presentation was skipped, due to time constraints.

11. DIALS & XIA2 – News, development, future directions (Graeme Winter)

GW gave an overview of software and other Dials developments. The recently awarded Wellcome Trust grant now pays three people, two of which are new hires (James Bielsten Edmands and Nicholas Devenish). The project will focus on scaling, integration of still shots, electron diffraction and performance improvements.

GW summarised current activities of the Dials team:

- implement basic scaling following XDS and Aimless (to ensure general approach)
- pointless-in-dials implementation
- performance evaluation

DIALS releases are frequent and time-, not feature-based. New features:

- xia2.report - general report generation tool given scaled unmerged MTZ
- Eiger support
- dynamic shadow masking
- static backstop masking via image viewer

New challenges ahead are:

- planned VMXi mode of operation, using a small and fast Eiger with many, many still shots; challenge on spot finding performance
- *in situ* data collection
- beamline commissioning with DIALS

12. DIALS GUI – Development and Demo (Luis Fuentes-Montero)

LFM gave an overview of changes since the last demo at WG2 (12.7.17). While the old DUI required mouse pointer navigation, the new DUI now features tree navigation to allow re-runs and forks. User proimts have been improved.

LFM then explained the implementation and use of the DUI, in three levels:

- The GUI allows the user to control iDIALS
- The iDIALS interactive shell is capable of running dials commands and navigate and grow execution tree; it can be used as a standalone tool, or be called from python code
- The command line tools used by iDIALS that are already available

The Image Viewer was built new, from scratch, and includes predictions overlap, different colour palettes, a video mode, stacked Images as new feature, a new HKL switch (On/Off), and “Google maps” behaviour. For the intermediate level, a new iDIALS mini shell was implemented that supports the new navigation behaviour. Navigation allows automatic mode that creates nodes on the tree and prompts suggests next steps, *vs.* an explicit node where the user controls all actions and creates nodes.

In the next couple of month, the DUI will be tested, receiving final touches before it is rolled out. WG2 was encouraged to test.

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

Possible date 24.1.2018, Location: London.

14. AOB

None.