



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 15th February 2017	Time: 11:00 – 16.00
Location:	Diamond House, Rutherford Lab, OX11 0FA, Oxfordshire, UK	
Circulation:	ccp4wg2@stfc.ac.uk	
Present:	Charles Ballard (CB), Dave Brown (DB), Nora Cronin (NC), Paul Emsley (PE), Gwyndaf Evans (GE), James Foadi (JF), Ronan Keegan (RK), Eugene Krissinel (EK), Andrey Lebedev (AL), Ed Lowe (EL), Marc Morgan (MM), Garib Murshudov (GM), Rob Nicholls (RN), Martin Noble (MN), Stuart McNicholas (SM), Robin Owen (RO), Paul Rowland (PR), Gianluca Santoni (GS), Kushwant Sidhu (KS), Kyle Stevenson (KS), Ville Uski (VU), Melanie Vollmar (MV), David Waterman (DW), Keith Wilson (KW), Marcin Wojdyr (MW)	
Apologies:	Arnaud Basle, Mike Hough, Karen McIntyre, Arwen Pearson, Christian Roth, Johann Turkenburg, Pamela Williams, Graeme Winter	

11:00-15:00 WG2 agenda

1. Approval of minutes from the London WG2 meeting 21/9/16
2. Chairs report (Ivo Tews)
3. Core group activities, CCP4 meetings and workshops (Eugene Krissinel, Charles Ballard)
4. Acta Cryst Proceedings Issue “Protein-Ligand Complexes” (Paul Emsley, Charles Ballard)
5. Acta Cryst Proceedings Issue “From Crystal to Structure” (Keith Wilson)
6. CCP4 study weekend 2017 “From Crystal to Structure” digest (Ivo Tews, Charles Ballard)
7. Data Processing Talks
 - a. Data collection and data processing (Gwyndaf Evans)
 - b. Data quality and error estimation (David Waterman)
 - c. Multi-crystal merging using hierarchical and genetic algorithms (Gianluca Santoni, ESRF)
 - d. Multi-crystal merging with the reciprocal space completeness scheme (James Foadi)
 - e. Emerging methods for multi crystal refinement (Garib Murshudov)
8. Discussion: proposed structure of the study weekend 2018 “Data Processing / Multi-xtal” (Ivo Tews)
9. Nomination for organisers and vote
10. Take note of the date of the next meeting (proposal 21. June 2017)
11. AOB

We will break for lunch during the meeting.

Minutes

1. Approval of minutes from the London WG2 meeting 21/9/16

The minutes from the London WG2 meeting 21/9/16 were approved.

2. Chairs report (Ivo Tews)

The primary function of WG2 is to oversee organisation of the study weekend and to support publication of the special issue as conference proceedings. The February meeting makes decisions on the topics set for study weekends, and recommends these to WG1. SW2018 will deal with multi-crystal techniques and data processing.

CB: we should make a note of the upcoming 40th anniversary of CCP4 – with special attention to the CCP4 study weekend.

WG2 are considering the best strategies for documentation and dissemination. The chair (IT) and the CCP4bb have received e-mails asking about the Wiki and a CCP4 pdf-type manual. There was also a discussion at the June meeting (2016) on teaching and potentially having a MOOC (online course). It might be an idea to bundle the current teaching material in an open folder accessible to all teaching the software / crystallography. Further advancing the Web-page to a modern design was discussed, and the possibility of funding this.

CB: suggested to approach STFC Media services to develop a front-end in WordPress; the costs for this would be moderate.

IT suggested considering all these documentation and dissemination streams for discussion with Exec and potential inclusion in the upcoming grant application.

It was noted that an open task is to have Jon Agirre presenting on Privateer.

3. Core group activities, CCP4 meetings and workshops (Eugene Krissinel and Charles Ballard)

EK reported on core activities. Release of CCP4v7.0 and maintenance is the most significant activity. There have been 30 updates so far through the continuous release model. Download patterns suggest that the update period is about once every six weeks. Release 7.1 is at an early stage of preparation and awaits input from external developers, such as code from PDB_REDO, WhatCheck, Molprobity, which needs integration.

For CCP4/Global Phasing, Marcin Wojdyr is now in post; he is tasked with updates on the mmCIF format in CCP4.

For GUI2 Liz Potterton has retired, and CCP4WG2 and core thank her for her involvement and efforts. Kyle Stevenson now handles management of GUI2; the work presently is focussed on bug-fixing. Kyle liaises with Martin Noble when needed. GUI2 is difficult due to time constraints of the core group, and the technical nature of the testing which does not allow automated procedures to test the code.

CCP4 activities around work package 2 of the grant on Molecular Replacement reported activities on ConKit, SIMBAD and further improvements in MrBUMP and AMPLE.

CCP4 activities around work package 0 of the grant on Cloud services are on-going and very successful. MN suggested to develop i2 pipelines as a backend of Cloud services.

CB reported on meetings: the past CCP4 Study Weekend, Nottingham (8-10.1.2017), and the planned ACA, New Orleans, USA, and IUCr, Hyderabad, India. CCP4 previously had a stand at ACA and IUCr; workshops: CCP4/Institute Pasteur South American School, Montevideo, Uruguay, 2017, 20 students; CCP4/Phenix, Hyderabad, August 2017; CCP4, Guangzhou, China. 23-27 October 2017, 20 students; CCP4-DLS, December 2017, 20 students; workshops and conferences where CCP4 is invited guest: Oulu, Finland, May 2016; Rapiddata, Stanford, April 2016; BESSY, Berlin, December 2016; Oulu, Finland, May 2017; Madrid, Spain, May 2017; Rapiddata, Stanford, April 2017; Electron crystallography, PSI, September 2017; CCP4 sponsored conferences: Northern Protein, Carlisle, August 2016; BCA-CCP4 Summer School, August 2016; SWSBC meeting, Portsmouth, Jun. 2016; Rapiddata, Stanford, USA, April 2016; ECM computing school, Lossberg-Wittendorf, Germany, August 2016.

4. Acta Cryst Proceedings Issue “Protein-Ligand Complexes” (Paul Emsley, Charles Ballard)

One part issue has been released and printed, some articles will follow in the next issue.

5. Acta Cryst Proceedings Issue “Crystal to Structure” (Keith Wilson, Charles Ballard)

We are on track presently with submissions, with a planned May deadline for contributions. It was noted that some of the talks and papers may not 100% correlate, and it was noted that some of the titles would require update (KSW).

The question was raised that we should have a new standard citation for CCP4. The suggestion was made that Liz Potterton should write this on the CCP4 GUI2 development. Direct further suggestions to KSW.

The question of an editorial was raised, DB to approach Dave Stuart.

CB floated the idea that the release of a pre-document might be an incentive for submission on time and allow authors who have written up on time to cite their work in advance of the release of the special issue. This was met with approval. CB to investigate.

6. Study weekend 2017 “From Crystal to Structure” digest (Ivo Tews, Charles Ballard)

The study weekend was a success and CCP4WG2 thanks the organisers Mike Hough and Keith Wilson for their efforts. The lunchtime-bytes were successful and sought after as ever. Particularly, DIALS and BLEND sessions were full. The format should stay as one talk per person.

CB reported a hack of the events booking system, with a new system coming up for next year.

7. Data Processing Talks

Data collection and data processing (Gwyndaf Evans)

GE covered DP requirements now and the future, going towards the design of fully automated synchrotron beamlines. In those settings, visualisations also become important, e.g. Apps for phones, tablets, etc. The trend is already to 70-80% of data collections being done automatically (defaults from prediction).

DIALS organisation and scope as a highly organized and highly modularized processing software that supports multiple detectors and experiment types. Joint refinement proves to be particularly useful in which multi-crystal data are treated.

The future will bring the handling of a large number of multi crystal datasets. Also, one would wish to see support for the neutron community with different type of detection and for electron diffraction experiments. Further development on the XFEL side. One should encourage developers from other sites (e.g. ESRF)

GE introduced I24 and the experience with micro crystals. There is an issue of managing waste: a better selection of datasets for EP/MR etc. DIALS has become a one-stop-shop for different techniques, methods, scenarios and detectors.

Data quality and error estimation (David Waterman)

Effort is needed in backward modeling, profile fitting and better error models. The focus on better data quality and error estimation is driven by better detectors that allow better error estimates – these are in fact urgently needed and possible. The question is out: How much can be learned from the small molecular community?

Multi-crystal merging using hierarchical and genetic algorithms (Gianluca Santoni, ESRF)

Techniques for multi crystal merging were covered by GS, demonstrating a novel genetic algorithm and a clustering method. The latter can be accessed via github.

Multi-crystal merging with the reciprocal space completeness scheme (James Foadi)

Novel developments on multi multi crystal merging in Blend were presented. First success in 2014 with membrane proteins. A novel reciprocal space viewing tool was presented, addressing data quality and completeness issues.

GE: the visualisation of data sets is a very important aspect. More tools are urgently needed.

Emerging methods for multi crystal refinement (Garib Murshudov)

Refinement against multiple types of data were covered, where experimental information comes from EM/NMR/X-ray. All these experimental techniques require different scattering factors and pose the question of relationships between different form factors. There are unresolved problems with EM and EC (electron crystallography) in terms of overlapping effects of charged atoms and solvent

ACTION: RN & GM – i2 needs to be kept up-to-date with refinement developments

8. Discussion of the study weekend 2018 “Data Processing / Multi-xtal” (Ivo Tews)

The meeting should cover methods in data processing, with appropriate treatment of multi-crystal techniques. Practice is automated data collection a.k.a. shoot first ask later. This leads to proposal for the following possible topics: (1) Processing on the fly; (2) Multi-crystal data sets, the norm rather than the exception; (3) reprocessing of data; (4) new sources and new intensities; (5) changed sample requirements, small and multi; (6) automated pipelines

MN suggested the program should focus on teaching and highlight new developments.

CB suggested that appropriate introductions should be given.

NC suggested there should be online talks to teach basics (see also 2)

A number of potential organisers were discussed and the decision was made by vote; IT to approach potential organisers and report back.

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

Possible date 5.7.2017 or 12.7.2017, Location: London. Google poll to follow.

10. AOB

None.