



# Agenda

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<b>Meeting title:</b>	CCP4 Working Group 2 meeting	
<b>Date:</b>	Wednesday 30th September 2015	<b>Time:</b> 11:00 – 16.00
<b>Location:</b>	Birkbeck, University of London, room 612 Malet St (entry from Torrington Square)	
<b>Circulation:</b>	ccp4wg2@stfc.ac.uk	
<b>Present:</b>	Jon Agirre (JA), Pierre Aller (PA), Charles Ballard (CB), Arnaud Basle(AB), Nora Cronin (NC), Paul Emsley (PEM), Phil Evans (PRE), Mike Hough (MH), Misha Isupov (MI), Ronan Keegan (RK), Nick Keep (NK), Eugene Krissinel (EK), Karen McIntyre (KM), Claire Naylor (CN), Stuart McNicholas (SMN), Marc Morgan (MM), Garib Murshudov (GM), Harry Powell (HP), Andrew Purkiss (AP), Christian Roth (CR), Paul Rowland (PR), Khushwant Sidhu (KW), Ivo Tews (ITE), Ville Uski (VU), Melanie Vollmar (MV), Helen Walker (HW), David Waterman (DW), Pamela Williams (PW), Graeme Winter (GW), Marcin Wodjyr (MW),	
<b>Apologies:</b>	Svetlana Antonyuk, Dave Brown, Kevin Cowtan, Judit Debreczeni, Eleanor Dodson, Gwyndaf Evans, Vilmos Fulop, Ed Lowe, Airlie McCoy, Arwen Pearson, Johan Turkenburg, Keith Wilson	

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Please arrive for coffee at 10:30.

Directions <http://www.bbk.ac.uk/geology/contact-us/how-to-find-us>

1. Approval of minutes from the Cambridge WG2 meeting 8/7/15
2. Chairs report (Ivo Tews)
3. What's new in CCP4 Core group, CCP4 6.5 Updates (Eugene Krissinel)
4. Gui2 roll-out (Jon Agirre, Eugene Krissinel)
5. Web pages (Eugene Krissinel)
6. Conferences and workshops (Charles Ballard)
7. Acta Cryst Special Issue "Phasing" (Charles Ballard)
8. SW2016 on **Protein-Ligand Complexes: Understanding Biological Chemistry** (Paul Emsley)
9. SW2016: What's new in CCP4, Lunchtime Bytes (Ville Uski)
10. Proposal for SW2017 topics, to be brought forward to WG1 (Ivo Tews)
11. AOB
12. Take note of the date of the next meeting (proposal 2.3.2016)

*13:00 – 14:00 Lunch*

1. DIALS – Overview and capability (Graeme Winter)
2. DIALS demo (David Waterman)
3. DIALS workshop (Graeme Winter, David Waterman)

*16:00 close*

# Minutes

## 1. Approval of minutes from the Cambridge WG2 meeting 8/7/15

The minutes from the Cambridge WG2 meeting 8/7/15 were approved.

## 2. Chairs report (Ivo Tews)

WG2 welcomes new members who have signed up; both receiving the mailing list and in attendance. WG2 focuses on “practicing crystallographers” in its constituency; while giving programmers the opportunity to discuss new developments, WG2 thus offers the option to discuss with users / the community. In this sense, it would be useful to more closely link users of Synchrotron sources, specifically DLS, close to operations of CCP4WG2. The advantages would be to get feedback on software us as well as identifying future needs. There is the option of contacting DLS bags through Diamond (rather than directly, because of data protection issues). The issue of modernizing web pages remains a target.

## 3. What's new in CCP4 core group, CCP4 6.5 (Eugene Krissinel)

Preparation for release of CCP4 7.0 are well underway; a test DL is available for all developers. The switch to i2 is urgent, and testers are welcome.

Major tasks for the core group include nightly builds and bundles. This requires a dedicated workstation; a fluent procedure to create bundles for all platforms is envisaged. While this presently focuses on Mac and Linux, the work for Windows is taken over by a new staff member (Kyle Stevenson), who is also essential for outstanding windows development of GUI2.

The release path: CCP4 6.5 goes through to Dec 2015. then CCP4 7.0 is branched; a code-freeze in mid November will allow release in mid December.

CCP4 7.0 Highlights include

- GUI2
- SHELX: to be included as binary
- DIALS: as the software is in rapid development, we are to experience frequent updates (this may be affected by the plan to change the build system for cctbx)
- Arcimboldo (light): presently in development
- MolProbity
- Whatcheck that is needed by PDBRedo will be added as update in CCP4 7.0
- Various Updates for existing software

Future development needs are viewing and summary tools for sequence annotation and structure.

## 4. Gui2 roll-out (Jon Agirre, Eugene Krissinel)

Gui2 was successfully tested at a workshop at St Andrews. The team also ran a demo at the ECM29 Advanced software development School Croatia. Both these tests received positive feedback and helped developing the software.

Most tasks now have documentation. Automated testing is being set up. New: a visual model prep tool using hmmer and chainsaw in MG (Stuart, Ronan). Work in progress: MG in HTML (Stuart); MrBump basic (Ronan); ARP/wARP (Andrey); Arcimboldo (Jon). Development going on in the background includes removing of redundant tasks as well as bug fixes (Liz, Stuart). The Task menu / toolbar, cleaned up list of tasks.

The main discussion centres on adding new tasks and wrapping more CCP4 programs - wrappers/task interfaces will have to be created. It was noted that while the interface is based around tasks rather than individual programs, several people would still want to use individual programs. Further discussions dealt with the co-existence of i1 and i2, and (database) migration of projects from i1.

#### 5. Web pages (Eugene Krissinel)

The overhaul of the web-pages was delayed since the effort to outsource this job was unsuccessful – CCP4 have approached two designers, but after initial interest these were not delivering. The question is now how this could be done – Eugene made clear that there is insufficient resource in core to do this.

The investment of CCP4 core is focused on CCP4-online and Web-services. Continued are MrBUMP, Balbes, Zanuda and JsPisa. The following projects are in the make or in final stages of preparation:

- AMPLE
- SHELX – test stage (with George)
- CRANKs2 - Utilization is at 90% (600-700 jobs per month, with ~100 active users per month). Change: 128 cores were recently acquired. Status: technical negotiations, services may become available to Diamond users.

Etan suggested hosting a TLS server.

#### 6. Conferences and workshops (Charles Ballard)

Increasing activities at workshops are a serious time commitment of CCP4 core and to developers. It would be helpful to be able to add lectures from non-developers - Charles suggests that suitable lecturers may be identified and nominated as “first choice person” on a given topic.

Past activities in last period;

- APS
- Madrid
- China (bi-annually)

Scheduled:

- Diamond workshop 1<sup>st</sup> - 9<sup>th</sup> December, deadline 16<sup>th</sup> Oct, 16-20 applications.
- Workshop in India (annually?)
- Uruguay

#### 7. Acta Cryst Special Issue “Phasing” (Charles Ballard)

The Acta Cryst Special issue has a number of papers already: six papers were accepted, two papers were transferred. From the list of speakers, we are presently missing responses / submissions from six speakers. The remaining manuscripts are in progress and a publication date in January is anticipated.

#### 8. SW2016 on Protein-Ligand Complexes: Understanding Biological Chemistry (Paul Emsley)

This will be held in Nottingham on 8<sup>th</sup> – 10<sup>th</sup> January 2016.

The invited speakers list was presented; speakers have all confirmed. The programme and planned talks were presented, the website is live. The programme had to be slightly trimmed to fit the timeframe, with not all talks being given half hour slots. The topic of fitting DNA and RNA had to be removed.

Presently: recruiting chairs; 70 registrations after 1st announcement on BB, another announcement to follow, Early bird registration closes 22<sup>nd</sup> November, registration closes 14<sup>th</sup> December.

Suggestion to also invite PDBe to the meeting, perhaps to include as a lunchtime byte (PME). Further, plans for the special issue was discussed, with the option that papers do not strictly have to follow the conference layout but must represent the topics covered, which could lead to reshuffling of authors and inclusion of authors that have not presented (ITE, seconded by Garib).

The discussion on possible CCP4 centred posters or flyers, as it was generally felt these should be available at the conference; promotion material could also go into delegate packs (CB). The suggestion was also plugging BCA membership/meetings at CCP4 (PW) – while CCP4SW is primarily about CCP4 activities and new software developments, advertising other groups would be OK (ITE). Should CCP4 offer flyers on a desk (ITE)?

### 9. SW2016: What's new in CCP4, Lunchtime Bytes (Ville Uski)

The following is planned for the CCP4 session 9-11:

- What's new in CCP4
- Special attention to ccp4i2 release
- intro and general use of i2
- Liz – more in Gui2
- Kevin
- Stuart

David (DW) and Graeme (GW) mentioned that in 2015, Xia2 was presented, and DIALS should be included this year. There was a general feeling that DIALS should be represented in this session.

Lunchtime Bytes: these should start 30 minutes after the lectures finish to allow for lunch. The system in the past with several speakers per session has caused problems; it would be essential to stick to times, perhaps these sessions could be more strictly chaired, however it may be good to get more rooms, and fewer speakers per session. Planned are:

- CCP4i2
- ccp4 and friends, to include, e.g.,
  - CCPEM
  - PdbRedo
  - PDBe
  - ccp4 web services
- archimboldo
- data processing
- molecular replacement

DIALS was suggested to run as the main hall lunchtime byte.

### 10. Proposal for SW2017 topics, to be brought forward to WG1 (Ivo Tews)

Four topics are in the running and have been suggested as possible SW theme:

1. From crystal to structure
2. Bioinformatics
3. Extending boundaries: low resolution, high resolution
4. Data processing

Discussion:

- (1) From crystal to structure. This topic was last presented 2010. In light of the Gui2 release, it is timely. It would produce a main paper of impact with many citations (ITE). Indeed, it would be an option to produce 1 big i2 paper and lots of papers on various methods (GM). Model building / refinement is up in the cycle, as it was last presented in 2011 (CB), and this could be covered in Crystal-to-Structure (ITE). Lots of new students are doing crystallography without having the appropriate background, so education and teaching is important (SMN). But workshops may be better for teaching (GM). However, there are hundreds of students who will never get to a workshop; we should always remember who the study weekend is aimed at - this was always students and other neophytes, rather than the old hacks who have been going since the dark ages and have seen it all before (HP).
- (2) Bioinformatics. The topic propagates the whole structure solution workflow, but as a sole topic is not seemingly popular.
- (3) Extending boundaries. Maybe joint ccp4em meeting (should be joint organised (NK)
- (4) Data processing. This topic was last covered in 2012. It might be early for data processing, as we are presently in a 6-7 years cycle (HP). DIALS is new and is felt needs some exposure, so organising a workshop on data processing was felt timely. With increasingly automated data collection and processing it becomes even more important to understand a bit of what goes on in the "black box" (HP). Agree - there's a lot of focus on the new & funky and awesome for corner cases stuff much less on the bread & butter that new folks to mx need; what happens when the automatic processing quits working (GW)? Data processing should include Multi-crystal data collection, processing and refinement, and cover, for example, sample prep/delivery/mounting, data collection strategies (static single shots, thin wedges ...) as well as data quality (AP). It may also include electron crystallography (HP).

Vote:

- (1) Bioinformatics: 0
- (2) Hi/low resolution: 6
- (3) \*\*\*Crystal to structure: nearly everyone in the room
- (4) Data processing: not quite as many as from crystal to structure.

\*\*\* Clear winner - so propose to WG1, done by Dave Brown. Organisers are to be nominated at next WG2 meeting, suggestions welcome.

## 11. AOB

None.

## 12. Take note of the date of the next meeting.

Proposed date 2.3.2016, Location: Doodle poll.

*The DIALS DEMO featured the current state, i.e. command line oriented, which requires typing tasks in order, and still following the scheme as designed in 2011 (good foresight!!) - demonstrated were: import - find spots - index - refine bravais lattice - refine - integrate - export mtz -> pointless/aimless.*

*The missing User Interface was discussed, as it will take a significant effort establishing this, but most people think this is a good idea. DIALS does not include decision making. as we have Xia2 for this, and in fact this is already in practice at DLS. David then gave a demo on DIALS.*