



# Agenda

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<b>Meeting title:</b>	CCP4 Working Group 2 meeting	
<b>Date:</b>	Wednesday 8th October 2014	<b>Time:</b> 11:00 – 16.00
<b>Location:</b>	London Research Institute (CRUK), Lincoln's Inn Fields Laboratories, Room 703B	
<b>Circulation:</b>	ccp4wg2@stfc.ac.uk	
<b>Present:</b>	Jon Agirre (JA), Charles Ballard (CB), Arnaud Basle (AB), David Brown (DB), Kevin Cowtan (KC), Airlie McCoy (AMC), Eleanor Dodson (ED), Phil Evans (PRE), Mike Hough (MH), Ronan Keegan (RK), Nick Keep (NK), Eugene Krissinel (EK), Andrey Lebedev (AL), Stuart McNicholas (SMN), Rob Nicholls (RN), Martin Noble (MN), Liz Potterton (LP), Andrew Purkiss (AP), Khushwant Sidhu (KS), Ivo Tews (ITE), Jose Trincao (JTR), Johann Turkenburg (JT), Keith Wilson (KSW)	
<b>Apologies:</b>	Paul Emsley, Rasmus Fogh, Garib Murshudov, Arwen Pearson, Harry Powell, Thomas Schneider, Roberto Steiner, David Waterman, Pamela Williams	

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1. Approval of minutes from the Cambridge WG2 meeting 11/06/14
2. Chairs report (Ivo Tews)
3. Membership and Preamble (Ivo Tews, Keith Wilson)
4. CCP4 SW 2015 "Phasing" (Airlie McCoy)
5. Proposals for CCP SW 2016, to be brought forward to CCP4 WG1 (Ivo Tews, Dave Brown)
6. What's New in CCP4 Core Group, The Cloud, Meetings and Summer Schools (Eugene Krissinel)
7. CCP4 support for meetings and Summer Schools (Dave Brown, Ivo Tews)
8. CCP4 Gui2 (Martin Noble)
  - a. Project progress (Martin Noble, Liz Potterton)
  - b. Incorporation of MrBump (Ronan Keegan)
  - c. Incorporation of CCP4MG (Stuart McNicholas)
  - d. Bug report system and distribution (Andrey Lebedev)
  - e. Introduction to the system (Martin Noble)
9. Ligands project and advances in Acedrg (Rob Nicholls)
10. The CCP4 webpages (Charles Ballard, Ivo Tews)
11. AOB
12. Take note of the date of the next meeting.

# Minutes

## 1. Approval of minutes from the Cambridge WG2 meeting 11/06/14

The minutes from the Leeds WG2 meeting 11/06/14 were approved.

## 2. Chairs report (ITE)

SW2014 “Complementary Methods”, Acta Cryst special issue. There were a total of 16 submissions. Several articles were early in, and revisions were made for print in summer; presently waiting for some late articles. With respect to coverage of the meeting, several expected articles were not coming in, and we had to decide over the summer to stop chasing these (sadly these are NMR, EM, EPR, no submission from the drug design session). To complete the issue, we additionally volunteered submissions from CCPEM and CCPN. Two articles were initially over 20 print pages in length, and the authors followed the suggestion to shorten these. The topics not represented in the meeting were addressed in the editorial. An open question remains how complementary information can enter the PDB. Costs of the print issue were estimated with over £30k (CB), which at this level was discussed to be too expensive.

Preamble published and web pages updated.

## 3. Membership and Preamble (ITE, KSW)

WG2 has the primary function to organise the study weekend in January, *the* meeting. However, CCP4 also oversees activities of schools and workshops, and serves as a conduit for users to tell CCP4 what’s needed, see also item 7. The context has to be to phase all ccp4 activities; these would include software roll-outs, the study weekend, teaching in workshops and the spread of courses (how many, where) and spread of topics, and aligning these with the developers meeting at Coseners, and with major conferences such as the BCA or ECM.

WG2 is in a good position to advise CCP4 on and to oversee how CCP4 interacts with the user community. It is recognised to build on this relationship and to get buy-in from the user community, also to shape new developments. The user community is encouraged to find things that aren’t good, bring them up in WG2, discuss and find consensus in WG2, and suggest changes, and this will be subsequently brought forward to CCP4 exec. Further, we will involve the user community via WG1.

The structure is now in place to coordinate these activities (see Preamble on web pages).

We then discussed the eligibility for WG2, which presently is PIs, EOs, and Crystallographers in UK based companies. AMC asked whether this would not limit the membership to long-term posts? And whether this should include shorter contracts such as PostDocs? DB asked whether the various  $\beta$  testers and the developers should be asked to participate? KSW suggested that the constituency should be more general and include all ‘active’ crystallographers (UK based). ITE suggested to have a wide distribution, and focus on active users, with overlap of the UK based Diamond MX users, to make sure that what WG2 does is widely known. KSW cautioned that 2 of present 3 WG2 meetings are predominately talking about the SW. He also suggested that people wont come to WG2 meetings that are local, they need to be easy to travel to, ans thus should be located central, e.g. London. AMC suggested to identify needs from the community to give participants a good reason to come to WG2 meetings; we also have options like early access to new software and information on upcoming software. DB said that the WG2 is an excellent option for developers who want to interface with users, and finally MN made the comment that not enough users are at the present meeting.

#### 4. CCP4 SW 2015 “Phasing” (Airlie McCoy)

A draft programme was presented by AMC, with many of the talks confirmed. WG2 congratulated Thomas and Airlie for an excellent programme. AMC pointed out that there was a strong steer by the organisers to have a good female representation in the speakers, but unfortunately this was not always possible.

The programme was approved. There was a discussion on two minor points: (1) the synchrotron session looked repetitive, and it the point was made that strong guidance must be given to these five speakers with the suggestion to exchange talks between speakers, and IT reported this had worked nicely in the previous year; (2) representation of (all) present used / offered software packages for phasing (i.e. SHELX, CRANK2, SHARP, SOLVE) was deemed desirable; however there was a clear consensus that the motivation for programming the CCP4 SW is not for promoting CCP4 software.

AMC said that perhaps it would be helpful if developers could congregate in a coffee area so that users can approach them; RK made the suggestion to let have speakers and programmers have color badges. IT/CB said that bursaries are still available, and this can be advertised.

#### 5. Proposals for CCP SW 2016, to be brought forward to CCP4 WG1 (Ivo Tews, Dave Brown)

Options discussed are (1) from crystal to structure (2) Bioinformatics (3) Extremes in resolution, low and high.

#### 6. What’s New in CCP4 Core Group, The Cloud, Meetings and Summer Schools (Eugene Krissinel)

**CCP4 6.5.0.** Pre 6.5 is now available to testers. Support for 64bit windows. Still waiting for some components before this can be bundled for release in December. Special features for Gui2 implemented.

**CCP4 Cloud Plans.** CCP4 cloud (work package 0), start 04/15; considerations:

Considerations

- Cost of development
- Cost of deployment
- Projection in future
- Running/Maintenance
- User Experience
- Graphical Front end – preferably GUI2
- Remote Desktop – NX licenses expensive
- Resources – 1000’s of users concurrently connected may cause problems

KC asked whether Google would fund project? EK responded that we need to guarantee long term stability and availability of the code.

#### 7. CCP4 support for meetings and Summer Schools (Dave Brown, Ivo Tews)

WG2 has the primary function to organise the study weekend and to oversee activities of schools and workshops. We discussed the two local conferences in the UK, the SWSBC and the CCP4 Northern Protein Structure Workshop in Carlisle. Some comments from the SWSBC are appended. The context was that Exec asked whether we are getting the best out of courses we organise and conferences we sponsor. We should look at feedback and ACT ON IT.

- Align Subjects
  - With Rollouts
  - With focus areas on major conferences
- Capacity Issues
  - Good spread of topics
  - Intelligence needed
- Support of Conferences
  - Local meetings for students are feeders to CCP4SW & propagate use of software
  - Offers at these conferences (talks/drop-ins/associated workshops)

Conferences to align activities with are iUCR, Gordon Conferences, Carlisle, Current Trends in Structural Biology, EGI-GEANT meeting in Amsterdam, CCP4 Workshops are held in Argonne and Tsukuba (Japan). Lunchtime bytes should be considered for local meeting (Carlisle/SWSBC) where possible as they are the best representation of the use of the ccp4 software.

## 8. CCP4 Gui2 (Martin Noble)

Aim of Project

- Accelerate the easy
- Facilitate the difficult
- Allow Xtallographers to think about what they are doing

**Liz Potterton**

- Crank/SHELX/CDE now integrated
- Testers currently are selected users on 6.4.5 but this will be expanded

**Ronan Keegan**

- Incorporation of MrBump - works

**Stuart McNicholas**

- Incorporation of CCP4MG

**Andrey Lebedev**

- Bug Report System & Distribution
- Work in Progress
- Perhaps could do with comments section & a "like" tab for people who encounter the same bug
- Mailing List

**Martin Noble**

- Hierarchical projects
- Ability to export/import projects (all required files are accompanied)
- Render colours (not configurable yet)

KSW suggested to a workshop in Nov/Dec to support testing.

## 9. Ligands project and advances in Acedrg (Rob Nicholls)

A new monomer library and monomer description generator based on COD, Improve quality of prior data and use of Use small molecule coord data; Initial testing done - ~ 10 million bond observations, 0.5 Million bond classes. In CCP4 jhbuild -> included in next CCP4 release.

## 10. The CCP4 webpages (Charles Ballard, Ivo Tews)

It was reported that the web pages need to be modernised; because of time constraints, this will be brought forward to the next meeting (action - ITE).

## 11. AOB

None.

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

Possible dates end of January (suggested: 22. or 28.1.2015). Locations suggested: London. Google poll to agree on date and location to follow.

**Comments on the SWSBC in Bath (2014):**

I enjoyed the meeting and would be very interested in future SWSBC meetings.

It was interesting to learn more about the CCP4 as I previously knew very little. I am not sure if presenting the list of new features was the best use of the CCP4 time slot. Perhaps a larger page of the abstract booklet could be used to summarise all the individual program features and then a more specific example of why the software is good as a large part of the talk? For instance an example in which it would streamline a work process and why you'd be mad to carry out this without CCP4.

The idea of allowing the program to update itself seemed to be very important though and that definitely sunk in from the talk.

Ben Yarnall, Southampton

I particularly appreciated the update from CCP4, I think the general overview is the best way to reach the wide audience that the conference covers. For example the young PhD students from our group found the CCP4 talk very boring, they don't understand what most of the programs are, and so most of it went over their heads. I'm also not a full time structural biologist, it's just one of the techniques we use in our group, and so the general nature of the update from CCP4 was the best format from my point of view. My one suggestion would be a longer Q&A session after the CCP4 update, specifically designed so people can ask more detailed questions, and if possible bring this update to the first part of the meeting so there is more time to catch CCP4's representative and ask him any questions that you thought of after the session.

I also wanted to mention that I noticed the lack of update from Diamond at the conference this year, and I was disappointed. If, like our group, other people are allocated overnight and weekend shifts at Diamond then this significantly reduces your contact time with the beamline scientists and means you don't get to hear as much about new and upcoming updates on the various beamlines. The updates from Diamond at the SWSBC gives our whole group the opportunity to see what's new at Diamond, and the opportunity to talk with the beamline scientists in a more informal setting where the pressures of data collection don't weigh on your shoulders. I hope it can be passed on to Diamond that they were missed and that they're attendance is much appreciated.

Thank you for all your efforts to keep the conference engaging and useful, although ours is a very multidisciplinary lab we always attend the SWSBC on mass, because we find it the best conference of the year, both in terms of experience, and value for money.

Anna Fuller, Cardiff University

I found the "What's new in CCP4" session very helpful. I think that this is really good.

However, I can see that a demo session, perhaps run more with junior lab members in mind, might be really good. This year, for example, I can see that CCP4mg might have been very popular. Maybe having this run alongside a poster session might be popular? This might be a good way of showing the value of the meeting to CCP4?

Nic Harmer, Exeter

Thanks for another terrific SWSBC. A really good blend of science, methods, software, industry developments and our successes. I don't really use CCP4 being more NMR so I found the overview useful and I think I can use more of its features in my work. However after the new facelift I think everyone will know the content very well, but perhaps not what it all does so I think some specific demos on a theme might be useful. The theme could change each year.

These demos could run into breaks for those specifically interested in more. The big screen in break periods is often forgotten but very useful. We've done that at CCPN.

Some young PIs have grown and developed with SWSBC and they now have good links/support with the X-ray community in this geographic area. SWSBC also supports/promotes new lecturers entering the universities in the south of England/Wales from elsewhere. This sense of community and belonging is important and SWSBC is pivotal to this as well as sharing our science and expanding our students' experience.

Community is important. Long may it continue.

Stuart Findlow, Southampton

It would be great to see what is upcoming in the pipeline in the medium term future in terms of new developments or potential directions.

Also, perhaps something worth thinking about is how CCP4 will integrate simulation resources in the future. Are there any good emerging gold standards, is this something the community would want ( I hope they do).

Christopher Pudney, Bath