



# Agenda

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<b>Meeting title:</b>	CCP4 Working Group 2 meeting and Gui2 demo	
<b>Date:</b>	Wednesday 11th June 2014	<b>Time:</b> 11:00 - 16.00
<b>Location:</b>	MRC LMB Cambridge, 2N1 80	
<b>Circulation:</b>	ccp4wg2@stfc.ac.uk	
<b>Present:</b>	Charles Ballard, Arnaud Basle, Airlie McCoy, Gwyndaf Evans, Phil Evans, Ralf Flaig, Ronan Keegan, Eugene Krissinel, Karen McIntire, Stuart McNicholas, Garib Murshudov, Harry Powell, Andrew Purkiss, Thomas Schneider, Kushwant Sihu, Jose Trincao, Ville Uski, David Waterman, Pamela Williams, Marcin Wojdyr	
<b>Gui2 demo:</b>	Andrey Lebedev, Liz Potterton	
<b>Apologies:</b>	Dave Brown, Tom Edwards, Rasmus Fogh, Vilmos Fulop, Chris Morris, Arwen Pearson, Roberto Steiner, Johan Turkenburg, Clemens Vonrhein, Keith Wilson	

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1. Approval of minutes from the Leeds WG2 meeting 23/01/14
2. Chairs report (Ivo Tews)
3. Debrief on the CCP4SW 2014 meeting - conference proceedings (Charles Ballard, Ivo Tews)
4. What's New in CCP4, role of CCP4 Gui2 (Eugene Krissinel)
5. CCP4mg (Stuart McNicholas)
6. Preamble for CCP4WG2 (Ivo Tews)
7. CCP4 supported meetings and Summer Schools (Ivo Tews, Airlie McCoy)
8. CCP4SW 2015 "Phasing" (Thomas Schneider, Airlie McCoy)
9. AOB
10. Take note of the date of the next meeting

Lunch will be served 13-14 in the LMB canteen.

We will run GUI2 demos in two groups:

- 1- Group 1 will run in parallel to the WG2 meeting in room 2N260, 11-13 (by invitation from Phil Evans)
- 2- Group 2 will run in the afternoon in room 2N260, 14-16 (WG2 group)

You will have to provide your own computer. Instructions for the download and install are in a separate mail.

# Minutes

## 1. Approval of minutes from the Leeds WG2 meeting 23/01/14

The minutes from the Leeds WG2 meeting 23/01/14 were approved.

## 2. Chairs report (Ivo Tews)

Took office on January 23<sup>rd</sup>.

Participated Cosener's Developers Meeting April 2<sup>nd</sup>-4<sup>th</sup>; presentations on new developments (e.g. Gui2, Dials, Ligands, CCP-EM, PDB deposition, amongst others).

Participated at the CCP4 Exec meeting: Exec asks core team to facilitate integration into the distribution and underwrites Gui2 development.

Presented preamble document to Exec, see pt6 below.

## 3. Debrief on the CCP4SW 2014 meeting – conference proceedings (Charles Ballard, Ivo Tews)

The following manuscripts have been received: (1) Biophysics – four submitted, either in revision or accepted; (2) SAXS – four submitted, either in revision or accepted; (3) new mounts – two accepted, two manuscripts to be submitted until the end of June; (4) EM – three under review; (5) Dynamics – one under review, two to be submitted until the end of June; (6) Drugs / Ligands: no submission.

As in last years, there were problems keeping the submissions to deadlines. Indeed, while it was (and to date of the meeting still is) not clear that all topics of the meeting are covered, two additional contributions were invited to complete the issue: one from CCP-EM (under review) and one from CCPN (to be submitted).

## 4. What's New in CCP4, role of CCP4 Gui2 (Eugene Krissinel)

Gui2 integration and testing are well underway, and in response to the request from Exec Anrey Lebedev is working on Gui2 full time.

CCP4 6.5.0 will be released in September 2014, and feature full integration of MG. Installs for Mac clusters presently cause some problems, and for the Mac-OS-X release, for technical reasons, a setup manager may be preferred over a \*dmg type installation (but both may be offered); OS-X installs are expected to be system independent and use tarballs, similar to Linux installs.

CCP4 6.5.0 will contain an optional Gui2 alpha release. This may require two parallel update threads, with the second thread, accessible inside GUI2, for GUI2 updates that are not coupled to CCP4 updates. This may be required as the status of Gui2 is alpha, requiring independent responses when updates become available.

The ensuing discussion on Gui2 covered the following points:

- the classic ccp4i should not be removed; Marcin Wojdyr stated that the size of Gui1 is only 3 MB;
- migration to Gui2 should not be forced: just make Gui2 attractive and people will come; Harry Powell stated that from experience with iMosflm, it is clear that people migrate when a new interface offers better usability, and we should expect the same for Gui2;
- both Gui1 and Gui2 can be run at the same time, but they have incompatible database structures, and individual projects must be in one or the other;

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- migration of project database from Gui1 to Gui2 would be rather difficult because of database incompatibilities; this is not an absolute no-go, but as this would be technically challenging and use a lot of time it would only be made available if the community voices a strong demand.

There are efforts to unify build systems from the CCPEM team. The ensuing discussion on CCPEM covered the following points:

- there were no concerns raised for the proximity / merger if this simplifies use / installs and makes the package attractive;
- there are licensing issues to be considered here as CCPEM must not "sell" the ccp4 component at a lower price than CCP4 does;
- presentation of CCPEM issues should be invited to the next WG2 meeting, and the discussion be brought forward to Exec.

### 5. CCP4mg (Stuart McNicholas)

Updates to CCP4mg were presented and demonstrated. Highlights include:

- a new display table to look at several structures simultaneously, clicking display options on/off;
- an overhauled ProSMART interface; however this currently requires the dev version of ProSMART;
- integration of the PISA interface - some fixes;
- the picture wizards can now be run on a single chain;
- various fixes included in this release.

### 6. Preamble for CCP4WG2 (Ivo Tews)

A preamble document has been prepared that would replace the statement "organises SW and meets more often than WG1" to define the role of WG2 at the interface between programmers and users. Aside of overseeing the organisation of the annual CCP4 study weekend, WG2 is to advise Exec on user demands:

- find out how we can provide a forum for CCP4 developers and feed back user demands;
- find out how we can comment on meetings and workshops;
- find out how we bundle all necessary information on Web pages.

The chair declared an interest to aim for a better overlap between WG2 constituency and user groups (e.g. regional centers or Diamond bags) – action ITE.

### 7. CCP4 supported meetings and Summer Schools

This summer, a number of CCP4 funded crystallographic schools have reported significantly fewer applicants (CCP4/BCA summer school, Summer School Ottawa, Hamburg Issc14 workshop), where in past these have been heavily oversubscribed, typically three-fold. While the reasons are not entirely clear, there are certainly courses offered this year that were oversubscribed – these are mainly from-protein-to-structure courses that offer hands-on experience. It is suggested to gather intelligence on this summer's courses in the next WG2 meeting what makes an interesting course, in order to focus support on the most thought after offers.

There are particular issues with the CCP4/BCA-summer school and the plan for a Diamond course, due to potential overlap in a situation where we already have too many places. However, there is an identified need to have the hands-on experience to integrate data collection, devising beamtime (which Diamond may well be

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prepared to do) and go full circle with structure determination. As there are currently conversations on this issue, it would be good to have this presented at the next WG2 meeting.

Overall, we observe a shift of interest, and it would be good for WG2 to analyse the reasons in order to foresee developments, rather than running behind. If we gather information now we can have a more informed discussion in the September WG2 meeting and then feed back to Exec in December.

Eugene Krissinel reported that crystallography is still on the rise in South America; the workshop in Brazil was a success with 2.5 fold oversubscription; next workshop scheduled for 2015 in Montevideo.

### **8. CCP4SW 2015 “Phasing” (Thomas Schneider, Airlie McCoy)**

Dates Thursday 8 to Friday 9th for the study weekend; Wednesday 7th for Diamond user meeting; venue is the East Midlands CC, Nottingham.

The scope of the workshop will be on structure solution by experimental phasing techniques, with an emphasis on use of derivatives in structure determination and validation.

The confirmed organisers are Thomas Schneider, Hamburg, and Airlie McCoy, Cambridge.

The format will be six 2 hrs sessions; each session will first cover some background material and then discuss current developments; the following topics for the sessions were discussed:

- A. Introduction to phasing
- B. Derivatives
- C. Methodological Aspects
- D. Radiation Damage
- E. Synchrotron Beamlines and Phasing
- F. Evolving methods (e.g. EM)

A detailed discussion on individual speakers and topics followed (not minuted here due to the preliminary character of the programme). An update will be given at the next WG2 meeting.

### **9. AOB**

Web pages to be updated with information on the CCP4SW 2015.

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

Possible dates end of September / beginning of October (suggested: Thu Sept 25<sup>th</sup>).

Locations suggested: London, DLS.

Google poll to agree on date and location to follow.