

WG2 Meeting : Birkbeck January 30th 2013

Chair: Arwen Pearson (AP)

Minutes: Ronan Keegan (RK)

Attendees: Arwen Pearson (AP), Eleanor Dodson (EP), Phil Evans (PE), Charles Ballard (CB), Stuart McNicholas (SM), Roberto Steiner (RS), Ville Uski (VU), Ronan Keegan (RK), Harry Powell (HP), Eugene Krissinel (EK), Nick Kepp (NK), Sidhu Khushwant (SK), 2 Others....

Agenda:

SW 2014:

The main item for discussion was the subject of the 2014 Study Weekend. Two candidates were suggested: Experimental Phasing (EP) & associated topics or Complementary methods. PE relayed Airlie McCoy's suggestion that EP should wait until 2015 when the new Diamond beamlines (long wavelength) are up and running. So it was agreed that the next two meetings should be:

2014 – Two way street - Complementary methods

- Nottingham 3rd, 4th, 5th Jan 2014
- SAXS and EM, Modelling, NMR (spectroscopy – element ID (XAFS)), neutrons, XFEL? coming back in to help solve crystal structures (AP) + Better modelling?
- Organisers: TBD
- Suggested inviting CCPEM, CCPN, CCPbiosim
- Speakers (3-4 max USA):
 - a. Suggest inviting CCP4EM, CCPbiosim, CCPN
 - b. TBD
- ACTION AP: to contact selected organisers.

PE suggested some notes for potential CCP4 SW organisers:

- Give explicit instructions to speakers about what to talk about
- Good speakers are important
- 3-4 speakers is about the maximum that can be afforded from the USA

2015 – Experimental Phasing – old methods, new sources (PE)

SW 2013: Feedback:

- Some complaints about lunches and standard of rooms.
- Acta D publication timetable – increased pressure on speakers to submit on time (March submission deadline)
- 2014: Half hour later lunchtime bytes to allow speakers/students to eat
- Selected Speakers were good
 - All present wish to extend their thanks to Pietro, Helen and Airlie for organising a great meeting
 - Started with easy talks and moved to more advanced topics
- David Blow fellowship students 2 Chinese, 1 Indian
 - Is it appropriate anymore?
 - To be raised at the next Executive board meeting
 - Possibly better to direct towards Africa/South American students
- Live Streaming:
 - PE watched it – worked pretty well
 - One problem was that you couldn't get to stream except when it was actually active i.e. during the sessions
 - CB: SSC slowed down its purchase – had to use cloud – single feed only
 - Some speakers didn't want their presentations to be streamed
 - Archived – need to be taken off line after 1 week
 - PE: URL link provided in CCP4BB email was not correct
 - AP: can we have a test card well in advance – before start of talks. ACTION CB to push for this next year
 - ED suggested that the contents of the streams are written out and used as an incentive to get speakers to submit papers. Guidance for referees/iUCR
 - Rate of publication is a problem – not enough new science, not very original. This is perhaps not the point of this publication. Organisers should be clear in their instructions – if article is not new content it should be a review report. Better guidance is needed for authors/referees/iUCR
 - What level should consultation with iUCR be at? ACTION: CB to report back on this at June WG2.

Future of WG2:

- AP expressed thanks on behalf of everyone to Phil for running it for so long
- Where to from here? Currently its main remit is the study weekend organisation. It used to be a developers forum but that has moved to the annual developers meeting.
- AP suggests that it should involve more workshop activities and be a showcase for new software developments. This meeting will include an MG session with Gui2 being covered in the June meeting in York. It was noted that the Gui2 event will be aimed at users and not developers.
- AP also suggested that it should move it off the York-Birkbeck-Leeds axis and visit other Universities. Leicester could be a candidate. Universities in Scotland should also be included (PE)
- HP pointed out that this was similar to the old CCP4 travelling road shows.
- The workshops will involve setting up computational facilities ahead of time. AP requested CCP4 core team support for future events (ACTION). An alternative is to ask all students to bring laptops?
- Next WG2 in York – June – to be coordinated with York and SW organisers – first week in June – provisionally Wednesday June 5th

RCaH BALBES Server:

The CCP4 core team has taken over the running of the CCP4 BALBES server on computational facilities at the Research Complex. The York server remains but it's not clear how it will be supported in the future. Other services (MrBUMP, CRANK) will be made available from RCaH in the future.

The (temporary) web address for the new server is:

- rcoison.rc-harwell.ac.uk/BALBESSERV/

In the near future this will be linked to from the CCP4 website.

AOB:

All present agreed that the new updates manager is great and that they are using it. Some minor issues were reported:

- One user reported that their csh script was changed by one of the updates. ACTION core team to investigate
- Mac issues – hard coded locations in the ccp4 setup script. Makes it difficult to have a shared disk installation of CCP4 if paths change from computer to computer.
- AMPLE – Rosetta is currently not a support package by the core team but assistance can be given to users if they need help installing it
- Minor issue with QTPisa

Actions:

1. AP to contact potential organisers for SW 2014 and to bring to their attention the “Notes for organisers” (see SW 2014 section above)
2. CB to request changes to SW stream system. Introduce test card so stream can be connected to before presentations take place
3. CB to decide on level at which iUCR should be involved in the CCP4 SW Acta Cryst proceedings. Also provide guidance notes for authors/referees. Will report back on this in June 2013 WG2 meeting
4. Core team to support computational setup at WG2 meeting software workshops. Next meeting in York June 2013 (GUI2)
5. Core team to investigate problem with ccp4 setup script (csh) being adjusted by update installer