



Agenda

Meeting title: CCP4 Working Group 2 meeting

Date: Wednesday 13th October 2022

Time: 11:00 – 13.00

Location: Zoom

Circulation: ccp4wg2@stfc.ac.uk

Attending:

We will break at least 5 mins around the full hour

1. Approval of minutes from March/April/June WG2 meetings
2. Chairs report (Ivo Tews)
 - a) WG2 report
 - b) WG2 call for a new chair
 - c) CCP4 grant plans
 - d) CCP4 SW2024 proposals for WG1
3. SW2023 “Data - Subtle details to big insights”
(Anna Warren, David Waterman, Christoph Mueller Diekman)
 - a) Scientific programme: aim, structure, proposed speakers
 - b) Special issue plans
 - c) Social programme
 - d) ED&I (Karen McIntyre, Melanie Vollmar, Jon Agirre)
 - e) Organisation (Karen McIntyre, Charles Ballard, Ronan Keegan, Ville Uski, Ralf Flaig)
4. CCP4 hosted or sponsored meetings
 - a) Meetings and workshops (Charles Ballard)
 - b) Northern Meeting (Briony Yorke, Ivan Campeotto, Jon Agirre)
5. CCP4 Core news (Charles Ballard, Eugene Krissinel)
 - a) CCP4v8
 - b) Core group
6. Take note of the date for the next meeting (proposal 11.01.2023)
7. AOB

Minutes

1. Approval of minutes from March/April/June WG2 meetings

Minutes from April have been approved. Minutes from March and June will be circulated to the mailing list for approval.

2. Chairs report (Ivo Tews)

a. WG2 report

We have a new rota of Science and Housekeeping meetings that are online and each take 2 hrs. We discussed whether we should want to meet in person again soon and agreed we will do this in 2023 in London (or another location). In 2022, we had done “housekeeping” meetings that cover core news, organisation of workshops and the Study Weekend in January, February, June and October. We had done scientific focus meeting in March and April (on AI, molecular replacement, and data processing). There was a search for a volunteer to organise a meeting in November.

b. WG2 call for a new chair

The current CCP4 grant is ending in 2024, and there was a call for nominations of a new WG2 chair for the subsequent period. Nominations should be made directly to the current WG2 chair or to CCP4Exec.

c. CCP4 grant plans

The incoming chair of CCP4 is expected to build on the successes of WG2 in the current grant period, which include: were oversight on organisation of the CCP4 study weekend, organisation local meetings, workshops and schools, in particular resurrection of the “Northern” meeting, the CCP4 documentation project, the CCP4 web page, support of CCP4cloud, and a mechanism for software inclusion called “Path of software into the suite” with more scientific presentations in WG2, as well as an increased frequency of WG2 meetings.

Plans for the next grant proposal are at an early stage. Ideas include Deep Learning methods from crystal structure solution to annotation; all Electron diffraction; other data sources/high resolution maps (CCP-EM as collaborator); Template-based modelling of protein glycosylation. Applications for MX, low resolution cryo-EM and AlphaFold; match and model dynamic structure information with experimental multi-state data models. CCP4WG2 is asked to contribute further ideas. CCP4Exec will discuss all proposals in a meeting in November that deals with aligning these ideas to shape a proposal that is to be submitted to the BBSRC in April 2023.

d. CCP4 SW2024 proposals for WG1

We discussed whether the CCP4 study weekend rota should follow the “classic” rota of meeting with the topics, which is roughly: data processing > phasing > molecular replacement > refinement > model building, followed by a crystal-to-structure or special meeting. It was felt that AF2 had changed the view on this, and thus that we would propose a more general crystallography meeting to WG1, with a focus area set for each year. However, it was felt that we need to not compete with other general crystallography meetings, and keep the USP of the study weekend, which is teaching and education in crystallography.

3. SW2023 “Data - Subtle details to big insights” (Anna Warren, David Waterman, Christoph Mueller Diekman)

a. Scientific programme: aim, structure, proposed speakers

The organisers showed the scientific programme, organised in six sessions. New are the plenary talks and a panel discussion on day 1, after the Diamond Light Source users meeting, and the poster session. For

students registering, they are asked whether they want to present a poster. Most of the speakers are confirmed. Each session should have an introduction (30 mins) followed by 20 mins talks. The sessions planned are

1. Fundamentals of crystallographic data
2. Fundamentals of the experiment
3. Choosing a source
4. Big data
5. Between the Bragg spots
6. A new structural biology era

The programme was discussed in detail.

b. Special issue plans

Conversations with speakers who have been told participating involves participation at the study weekend.

c. Social programme

There will be games and a mixer, organised by Sam Horrel.

RN: Most of the ideas may come after the meeting, so probably important to catch that right after the meeting.

d. ED&I (Karen McIntyre, Melanie Vollmar, Jon Agirre)

A framework for this is now in place and comes up on registration.

e. Organisation (Karen McIntyre, Charles Ballard, Ronan Keegan, Ville Uski, Ralf Flaig)

No foreseeable problems, and we have to be out of the building at 5 pm.

4. CCP4 hosted or sponsored meetings

a. Meetings and workshops (Charles Ballard)

Presence at IUCR ECR Paris and Ben Gurion University Israel. Planned are ASCA in person, DLS meeting in person, Israel and APS, all in person. Some talks may be virtual, but in person talks are strongly suggested. Planned for 2023 are two local meetings for students and ECR, namely St Andrews Summer School in 2023 in York and the SWSBC July 2023 Southampton. Possibly good to see how people respond to virtual talks.

b. Northern Meeting (Briony Yorke, Ivan Campeotto, Jon Agirre)

The Northern Meeting has CCP4 support and now also several sponsors, close to 100 people attending, sixteen talks, with ten posters planned

5. CCP4 Core news (Charles Ballard, Eugene Krissinel)

a. CCP4v8

V8.0.005 out, 006 coming imminently for patch and coot issues, plus a cycle of updates that are in preparation for some time now. In March 2023 there may be a new release including new Python and use 3.10 DIALS. For coot, GTK4 implementation is being prepared by Paul, but there are performance issues on Mac that need addressing. Multiplex: work in progress to tidy up the interface; Pairref: likewise, some testing needed; DUI2 will be trialled at the DLS workshop to understand what the release date would be.

b. Core Group

GTK3 Coot does work on Mac, which will be released, there will also be two builds for Mac for the different architectures. We have AF functionality, for example fully integrated in CCP4*cloud* and in the automatic pipelines. Oleg has departed and Maria Fando has received a job offer to start.

6. Take note of the date of the next meeting

Proposed date: proposal 11th January 2023, online.

7. AOB

None.