



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Thursday 12 th January 2022	Time: 13:00 – 15.00
Location:	Zoom	
Circulation:	ccp4wg2@stfc.ac.uk	
Attending:	Jon Agirre (JA), Arnaud Basle, Paul Bond, David Briggs, Ivan Campeotto, Lucrezia Catapano, Kevin/Kathryn Cowtan (KC), Phil Evans, Maria Fando, Ralf Flaig, Luiso Fuentes Montero, Vilmos Fulop, Robbie Joosten, jpt3, Ronan Keegan, Petr Kolenko, Eugene Krissinel, Andrew Lebedev, Gustavo Lima, Ed Lowe (EL), Martin Malý (MM), Airlie Mc Coy, Karen McIntyre, Peter Moody, Christoph Müller-Dieckmann, Garib Murshudov, Andy Purkiss (AP), Dan Rigden, Mark Roe, Alan Roseman, Mark Roe, Paul Rowland, Adam Simpkin, Roberto Steiner, Ivo Tews, Ville Uski, Sameer Velankar, Clemens Vonrhein (CV), Anna Warren, David Waterman, Pamela Williams, Martyn Winn, Marcin Wojdyr, Briony Yorke	

We will break at least 5 mins around the full hour

Starts 13:00.

1. Approval of minutes from Oct WG2 meeting
2. Chairs report (Ivo Tews)
3. SW2023 “Data - Subtle details to big insights” meeting report (Anna Warren, David Waterman, Christoph Mueller Diekmann)
 1. Meeting report (Ivo Tews)
 2. Experiences and feedback (Anna, David, Christoph)
 3. Plans for the Acta D Special issue
4. SW2024 discussion
5. Core group news (Eugene Krissinel, Charles Ballard)
6. New CCP4 grant (Ivo Tews)
7. Take note of the next meeting (proposed 8th February 2023)
8. AOB

Minutes

1. Approval of minutes from the online WG2 meeting 13/10/22 (Ivo Tews)

The minutes from the online WG2 meeting 12/10/22 were approved.

2. Chairs report (Ivo Tews)

Reports to the CCP4 exec are due, and WG2 has had important roles in (1) organisation of the study weekend, (2) organisation of local meetings and workshops, (3) CCP4 documentation, (4) the ccp4 web page, (5) the CCP4*could* project, (6) the path of software into the suite and (7) now runs with an updated meeting rota. Indeed, we have had WG2 meetings on organisation the Study Weekend and workshops with reports on core activities in January, February, June and October, and also had scientific focus meetings in March and April (on AI, molecular replacement, and data processing). However, a scientific meeting in November did not take place as we were missing a volunteer to organise this. These activities were reposted to CCP4exec in November and at the study weekend in January to the CCP4WG1 group.

3. SW2023 “Data - Subtle details to big insights” meeting report

CCP4SW 2023 was overwhelmingly seen as a great success, and the new elements such as poster session, plenary, and panel were welcome novel elements. CCP4WG2 thanks the organisers Anna Warren, David Waterman, Christoph Mueller Diekmann. Problems with timekeeping were noted, as the program was full and did not allow enough wiggle room to cope with sessions that overran. Attendance was high, with 220 on site and between 300 and 400 unique users on each day.

JA: Superb meeting! Lots of new ideas. Loved the format.

EL: Excellent meeting. A very good balance of novel research and didactic content.

AP: Too many panel members, so not enough time each.

JA: Needs fewer panel members to get panel-audience interaction time.

RS: I would consider injecting some senior postdoc presence. Total 4 people 1 of which a senior postdoc

The hybrid meeting format received heated discussions. In particular poster session and social activities were discussed. The consensus was that it is difficult to make these activities work online. Problems with connectivity / WiFi were noted and should be fed back to the conference host.

KC: Board games were great. If I was virtual I would have been crafty instead. Someone with BoardGameArena experience who is not present at the meeting could lead people into online boardgames.

MM: I don't like the idea of virtual posters. I like how it was.

CV: Maybe allowing posting posters online/slack would allow students providing those at the last minute (no need for finding printer etc)?

RF: Posters could be uploaded to Slack. That would keep the organisational effort smaller.

PM: on line posters are more of a challenge to interact with the presenter.

JA: Just a thought: online/remote posters don't need to be posters. EBI/PDB meeting handled these great via zoom links. Needs standalone session.

AP: One issue with the hybrid format is that questions from remote people seem to get ignored in favour of people in the room.

PB: I found it difficult to engage properly with people in person and online at the same time during the hybrid lunchtime byte. I think having an in-person and a separate online session would have worked better (but takes more time). For slack, one option would be two slack channels: one for chat and one for questions.

Anna, David and Christoph reported for the organisers team. The organisers did enjoy organising this mean. The meeting met enthusiasm, with quick replies from speakers. Sam Horrel was brilliant to add the social framework, and poster session and games were well received. Activity in slack channels also had activity, crafty crystallographers worked, but online games did not work. The céilidh was missed. Also, it felt that not all information was not passed on on social activities, submission of posters, the poster prize, or signage for LTB sessions or the quiet room. For the panel, the interaction with between panel and audience was not ideal, but the panel discussion itself was successful, but could be more focussed (hot topic). Talks were varied in length, which seemed to work well, but the open question is whether all talks should be delivered in person. And the mix of educational and science content worked well. The combination of having two chairs, one young person and one more experienced one seemed to have worked well.

IT: There should be a collection of lessons learned that is passed on to the next organiser team.

CB: WG1 was squeezed and we need to provide space for that.

For the Acta D, we have a number of intended submissions. There are few that need to be confirmed whether they can submit. The number of articles is between 15 and 23.

IT: Does this represent the breadth of the meeting? Are all these articles going in on scientific merit? If some are educational, they should still be published, but editor and referees need to be aware. Timeline should be end of February to affirm all this and have submissions, which the scientific organisers can help with.

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4. SW2024 discussion

We discussed that the next SW would be a general meeting, but should look for a focus topic. It should focus on new methods, and one idea that gained some traction was to focus on automated vs. manual.

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

The imminent release is v8.0.008, to include Coot (0.9.8.7), iris (0.2.1), shelxe, shelxl, jscofe (1.7.009) and ccp4i2. This follows from earlier releases v8.0.007 that included Coot (0.9.8.6), mrparse, refmac, jscofe (1.7.008), ccp4i2 (2.0.06) and crank2; v8.0.006 that included Coot (0.9.8.5) and ccp4i2; v8.0.005 that included Dials (3.8.7), monomers, jscofe (1.7.007), ccp4i2, arcimboldo and acedrg. The release planned for summer will include python 3.9/3.10, and other major changes, such as updates on Dials, coot Gtk3/4.

The Northern meeting was a success. On workshops, the Diamond workshop end of the year well organised and a high number of applications (did admit 25), the AsCA conference in South Korea was also well attended as well. Planned are an APS workshop end of March, a meeting in Croatia, and potentially Thailand.

There was a fault on jisc to unsubscribe users from the CCP4BB but this is being fixed, apologies.

6. New CCP4 grant (Ivo Tews)

The present ideas for the new grant, to be submitted in April 2023 to the BBSRC. The proposal includes 4-5 WP and comes from the LMB, DLS, STFC, as well as Liverpool and Southampton Universities. Ideas from the early stages are now affirmed, and the WPs are currently being fleshed out.

7. Take note of the date of the next meeting.

Proposed date: proposal 8th February in London (hybrid).

8. AOB

None.