



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 8 th June 2022	Time: 14:30 – 16.30
Location:	Zoom	
Circulation:	ccp4wg2@stfc.ac.uk	
Attending:	Jon Agiree, Charles Ballard (CB), David Briggs (DB), Ivan Campeotto, Kevin Cowtan, Paul Emsley, Ralf Flaig, Ronan Keegan, Eugene Krissinel, Airlie Mc Coy, Karen McIntyre, uiso Fuentes-Montero, Peter Moody (PM), Christoph Müller-Diekmann, Paul Race, Dan Rigden (DR), Ivo Tews, Ville Uski, David Waterman, Anna Warren, Graeme Winter ← not the complete attendance list taken, apologies.	

We will break at least 5 mins after Pt.1

Starts 14:30.

1. Approval of minutes from the WG2 meetings 26/03/22 and 27/4/22.
2. Chairs report (Ivo Tews)
3. Study Weekend 2023 “Making the most of your data”, scientific programme
(Anna Warren, David Waterman, Christoph Mueller Diekmann)
4. Study weekend planning (Karen McIntyre, Charles Ballard, Ronan Keegan, Ville Uski, Ralf Flaig)
 - a. Venue; meals; ED&I
 - b. LTB
 - c. Social programme
 - d. Satellite meetings: DLS, WG1, EXEC, What’s New
5. CCP4 hosted or sponsored meetings
 - a. Meetings and workshops (Charles Ballard)
 - b. SWSBC Southwestern Meeting (Paul Race)
 - c. Northern Meeting (Briony Yorke, Ivan Campeotto, Jon Agirre)
6. CCP4 Core news (Charles Ballard, Eugene Krissinel)
 - a. CCP4v8
 - b. Core group
7. Take note of the date for the next meeting (proposal 27.07.2022)
8. AOB

Minutes

1. Approval of minutes from the WG2 meetings 26/03/22 and 27/4/22 (Ivo Tews)

The minutes from the online WG2 meeting 27/4/22 were approved. Minutes from the meeting 26/03/22 will be approved at a later stage through e mail circulation.

2. Chairs report (Ivo Tews)

The CCP4 documentation (Maria Fando) continues with funding to Newcastle with development on CCP4i2. A m/s has been submitted for the web based, portable learning system CCP4cloud. The post in serial crystallography is funded and should start in October 2022 in Southampton together with the Diamond Light Source.

The rota of WG2 meetings has seen meetings in January, February on “housekeeping” such as workshop and study weekend organisation and core activities, and in March and April on scientific topics AF2, molecular replacement, and data processing. This is to be continued at a similar frequency and split, generating a rota of short (2hrs) online meetings.

3. Study Weekend 2023 “Making the most of your data”, scientific programme

The consensus from discussions in WG1 and WG2 were to create a SW on experimental data that is integrative. Aspects that were suggested were crystallisation/crystallisability, sample delivery/prep including ssx, time resolved, sample prep for mx, em, saxs, ed and possible future capabilities at SR and Xfel sources. We recognise the increasing level of automation which is a problem for education. With the SW, thus, we want to give students a chance to listen to discussion between experts in a way that doesn't happen in a training school/workshop environment.

The meeting should provide opportunity to learn about software and instrumentation developments and theoretical underpinnings. The brief to the organisers team was to explain how good data look and how to best use Them, bringing the focus back to experiment and information beyond the model. As many PIs using structural biology may not be crystallographers there ought to be continued focus of the study weekend on education. Envisaged are introductory lectures, coupled with case studies and reports on novel developments.

The organisers Anna Warren, David Waterman and Christoph Mueller Diekmann then presented a first sketch of the meeting, which was discussed in WG2. Because there was a delay in appointing organisers, the organisers team had very little time to prepare this. Despite this, they presented several good ideas which were well received, planning 6 to 7 sessions with 2 * 30 min talks and several shorter talks.

On the first day that is normally reserved for the DLS users meeting, the proposal to have a discussion panel to discuss “A bright future for structural biology”. This would be opened with a talk that combines several methods to integrate across a biological problem.

The meeting across two days could have six sessions:

- Fundamentals of crystallographic data
- Fundamentals related to samples and the experiment
- Choosing your source
- Big data
- Between the Bragg spots
- A new era in structural biology

In “Fundamentals of crystallographic data”, the concept data would be defined, data processing from raw data (images) be described, and measures of data quality introduced. The session should include state-of-the-art methods of X-ray data scaling and treatment of multiple data sets, as in isomorphous clusters, SSX, time series, ligand screens, or in choosing the best single dataset from redundant collections.

“Fundamentals related to samples and the experiment” would include aspects of sample preparation, sample delivery, radiation damage, data collection strategies, and review automated data processing pipelines. Ancillary techniques (spectroscopy, HP etc.) and BioSAXS, CryoEM, CryoET may come into this as well.

“Choosing your source” would cover choice of structural biology technique to match the scientific problem, or the choice of beamline. It could be interesting to cover what different parameters mean (brightness, brilliance, divergence, bandpass / pink beam, tunability, experimental capability). We should also cover capabilities of modern X-ray detectors, spanning over concepts such as integration vs counting, DQE, count rate limit, or efficiency at different energy ranges. Capabilities of a modern “home source” are also a valid topic. Electron diffraction should be covered.

PM: Should we discuss deposition/storage/availability of “raw” data?

DB: Presenting the capabilities of a modern home source is timely, given that many European synchrotrons have significant dark periods in the next 4-5 years.

“Big data” deals with exascale computing, for example in SFX data processing or serial crystallography. Robust statistics and machine learning would be included. Time-resolved crystallography that requires this kind of advanced data storage and treatment sits well in this session, as do the giant datasets in CryoEM, CryoET if permitted. Multi-dataset density and structural analysis and preprocessing of SFX data are further interesting topics.

The session “Between the Bragg Spots” should go beyond the normal case, and could feature incommensurately modulated protein crystals, detection of problems with X-ray data, or pathologies. The latter might generate a particularly useful SW publication. Finally, observation of dynamics in proteins from diffuse scattering would be interesting to cover.

The final session should credit “A new era in structural biology”. We can cover the latest advances from CASP15, the EBI AFDB, protein dynamics, combined approaches and time resolved work, or the acceleration of structure solution through AI.

4. Study weekend planning (Karen McIntyre, Charles Ballard, Ronan Keegan, Ville Uski, Ralf Flaig)

- a. Venue; meals; ED&I
- b. LTB
- c. Social programme
- d. Satellite meetings: DLS, WG1, EXEC, What’s New

WG2 affirmed the ED&I agenda is in place, and users registering to the meeting will find a code of conduct and code of ethics. The run of LTB was discussed, as well as appointing a social organiser to help the team of scientific organisers. The framework program is to include the mixer on day one, which runs parallel to the poster session (new!), and activities thereafter – an idea would be a games night. The question how we would cater for an online attendance, and what the offer would be, was discussed. The scientific programme provides slots for the DLS satellite meeting on the first day of the meeting, as before COVID when meetings were held at Nottingham. The fact that we have a panel discussion on the evening could mean that we have good attendance numbers at the users meeting. Further, higher attendance at the WG1 meeting is expected, and the panel members are PIs themselves who would also be able to attend. Ville is in charge to organise the What’s new session.

5. CCP4 hosted or sponsored meetings

- a. Meetings and workshops (Charles Ballard)
- b. SWSBC Southwestern Meeting (Paul Race)
- c. Northern Meeting (Briony Yorke, Ivan Campeotto, Jon Agirre)

Charles covered plans for meetings and workshops, many of them now returning to live participation (post Covid).

The SWSBC Bristol 2022 planning is well underway, with many registrations already. Paul Race explained the plans for the two days meeting which is focussed on student and ECR participation, with a few PI talks as anchors in the six sessions. There is a social (conference dinner) and exhibitors are present at the meeting, some of which are invited to present. Further, CCP4 is asked to participate; Maria Fando will present CCP4*cloud* and Kyle Stevenson will present CCP4i2. Both will cover documentation.

The Northern meeting will also go forward, for a long time in a while. The structure is similar to the SWSBC meeting and facing students and ECRs, and will also have exhibitors.

Both SWSBC and the Northern meeting are supported through CCP4 funds.

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

- a. CCP4v8
- b. Core group

Charles and Eugene presented core activities.

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

Proposed date: proposal 27th July 22, online.

8. AOB

None.