



Agenda

Meeting title:	CCP4 Working Group 2 meeting	
Date:	Wednesday 29 th January 2020	Time: 11:30 – 16.30
Location:	Birkbeck B62, University of London, Malet Street, Bloomsbury, London WC1E 7HX	
Circulation:	ccp4wg2@stfc.ac.uk	
Signed up:	Jon Agirre, Danny Axford, Arnaud Basle, Dave Briggs, Gabor Bunkoczi, Kaushik Hatti, Mike Hough, Louise Jones, Ronan Keegan, Nick Keep, Ed Lowe, Karen McIntyre, Stuart McNicholas, Rob Nicholls, Nikos Pinotsis, Andrew Purkiss, Randy Read, Dan Rigden, Paul Rowland, Mark Roe, Alan Roseman, Kyle Stevenson, Roberto Steiner, Ivo Tews, Ville Uski, Melanie Vollmar, Keith Wilson, Graeme Winter	
Apologies:	Pierre Aller, Svetlana Antonyuk, Charles Ballard, Dave Brown, Agata Butryn, Tristan Croll, Vilmos Fulop, Robbie Joosten, Eugene Krissinel, Andrew Lebedev, Garib Murshudov, Pietro Roversi	

Directions: Come to the [main Birkbeck entrance](#) go as far right (North) on the ground floor as possible (head for lift B). Use the phone by the door ahead of you to ring 6800 to be let in to 'crystallography'. Follow the corridor and then go down the stairs. Two right turns will get you to B62 (Glaxo-Wellcome) Room.

Please arrive for coffee at 11:00; we will start 11:30 and break for lunch at 1:30 pm

11:30-16:30

1. Approval of minutes from the London WG2 meetings 26/09/19
2. Chairs report (Ivo Tews)
3. CCP4 SW2020 "Model building", feedback (Ivo Tews)
4. CCP4 activities, workshops, roadshows (Ronan Keegan, Keith Wilson)
5. CCP4 SW2020 proceedings (Jon Agirre, Alan Roseman)
6. CCP4 SW2021 "Integrating Structural Biology", planning, appointment of organiser team (Ivo Tews)
7. CCP4 – news for publishing the virtual special issue, discussion (Lousie Jones, IUCr)
8. New Software:
 - a. What's new in CCP4 (Kyle Stevenson, Ronan Keegan)
9. Serial Crystallography (Ivo Tews)
 - a. DIALS goes serial (Graeme Winter)
 - b. The serial crystallography experiment (Mike Hough)
 - c. Processing serial data – what's missing? (Danny Axford)
 - d. Dynamic crystallography bag at Diamond (Danny Axford)
10. Take note of the date of the next meeting (proposal 20th May 2020)
11. AOB

Minutes

1. Approval of minutes from the London WG2 meeting 26/9/19 (Ivo Tews)

The minutes from the London WG2 meeting 26/9/19 were approved.

2. Chairs report (Ivo Tews)

WG2 reported to WG1 in January as part of BBSRC grant for outreach and impact activities. A question that came up from WG1 was whether three WG2 meetings are sufficient (they presently are), if not support by WG1 was volunteered. For considering new software WG2 provides an excellent forum. WG2 discussed how we could reach out to future developers. We may help to get novel software into the suite through the WG2 route, and by showing a slide at SW plus information or a special page on the website to clarify this route exists. We should also make clear to non-CCP4 developers what libraries are available. We could send an invite out on bb and make further announcements at computing schools, however, must be mindful that non-crystallographic software puts an extra burden on the core team. The CCP4v7.1 is already 5 Gb in size, which we must also be mindful of.

The issue of childcare at Study weekends was discussed. Looking at possibly bringing it in for SW2021 but need to be looking at this at the next WG2.

The Webpage has some technical glitches that at present prevents launch. IT reported some content is also in the process of revision. VU and IT to discuss and Dave Brown send strong e-mail to STFC regarding this.

WG2 discussed what the reasons were that citations were going back. CCP4 offers a super refinement engine, a fantastic interface, an exceptional ligand treatment, and is scientifically leading. Success of our software must reflect in citations, as future funding for the science we do depends on it! It was discussed that the phenix interface was preferred by many users over CCP4 GUI2. For refinement, people may use Refmac for routine jobs using the speed of the engine, but then finalise and deposit structures with phenix.refine where validation is easy and refinement satisfies criteria better - users will always go for lower R factors and less reported outliers. Currently we use molprobity, and the question was whether we may need alternative validation tools. New validation/deposition tools, the ligand SW, and a very active ligand group with new dictionaries are important to get more deposition citations. Recognising this, deposition is being made easier with the coming v7.1.

However, we need to identify further issues that make use of the software even easier. We should ask users what they need/require, engage PI's, and learn from teaching students or novices. Workshops, roadshow and presence at meetings are recognised as significant activities that help and improve on distribution and use of the software. Promoting the suite must be a priority for getting people to use CCP4 software.

A further issue discussed was user support, and if a problem is identified by users than -regrettably- they may not contact the core team or the developers. The update cycle also takes long. The phenix team are able to respond to requests for updates quickly, and they supply beta versions for new software on user request. Whether there can be a change to the approach in the update can be discussed with the core team. Another way forward is the move to Cloud solutions (coming).

One question that came up: Are there too many tools in the suite, and can we take out the non-core elements, or have them as optional. This may give the impression of CCP4 not being focused, while phenix has a more integrated vision.

3. CCP4 SW2020 “Model building”, feedback (Ivo Tews)

CCP4WG2 congratulates the organisers Jon Agirre, Robbie Joosten, and Alan Roseman! The 2020 study weekend was seen by all as a fantastic meeting. We had overwhelmingly positive comments. Good points mentioned included the many new ideas at the meeting, ie. quiz, stickers for matching interests, and the competition for poster / cover (although for the latter several people remarked that better advertising was necessary as they hadn't known about it).

For the programme, the buffer for discussion worked well to keep the meeting on time. The talks were remarked to be more idea based which was seen as positive for students to think conceptual rather than simply having a math-based programme. The ever-changing topics in the talks meant the program was never boring. The lunchtime-bytes worked well. Streaming worked well – higher resolution, feedback very good!

Negative points. There were too many talks, there was too much EM in the programme, The MR clinic was missing out – advertising required. The competition screens were overlooked.

4. CCP4 activities, workshops and courses (Ronan Keegan, Keith Wilson)

Impact of these activities should be to promoting use of CCP4, to educate researchers on best practice, and to help researchers to solve their target structure by hands-on-expertise. The benefit are use of and citations for the software. Workshops just finished or planned are as follows:

- DLS December 7-15
- AsCA, Singapore December 17-18
- SEACOAST, Bangkok, Jan 22-29
- Israel, Feb
- South Africa, Feb
- Madrid
- Rapiddata
- BCA summer school Norwich
- APS, Chicago, Jun 15-22
- SWSBC June
- IUCr, joint CCP4/CCPEM, Aug
- Uruguay, Sept
- Spring-8, Japan, Oct start
- India, Oct/Nov?
- Shanghai, Oct?
- DLS Nov
- DLS bag training (contribution)
- GRC (sponsor)

The call for speakers if you are interested is always open – the core team welcome help at workshops.

The 1 day CCP4 roadshows can now be rolled out, too, and they are an excellent opportunity to feature the software and i2, contact Keith. Planned are Oxford, York, Newcastle and Birkbeck. Roadshows typically take 2-3 hours and so far have been well-received.

Additional ideas extend to the use of Webinars, possible by using zoom (eg.), and we could do videos and have a YouTube channel. Stuart Mc Nicholas is happy to take suggestions and help. These would serve as additional teaching materials rather than replacement for roadshows.

5. CCP4 SW2020 “Model building”, Special issue (Jon Agirre, Robbie Joosten, Alan Roseman)

All contributors to the 2020 study weekend have agreed to contribute a manuscript to the special issue. Jon will give an update at the next WG2 meeting.

- 24 people with intention to submit – no-one has said no!
- Papers divided over 3 organisers who will act as editors
- Sent e-mails – some have replied

6. CCP4 SW2021 “Integrating Structural Biology”, planning & organiser team (Ivo Tews)

There is scope to include all structure giving techniques - X-ray (crystallography, SAXS), NMR, EM. Further, we would include complementary techniques (biophysical techniques). Finally, bioinformatics, MDM & structure analysis should be part of this meeting. Deposition of complex data is an issue we probably need an informed view on.

A study weekend also gives opportunity to feature new CCP4 developments; check against new grant deliverables such as electron diffraction. We should look at overlaps with other CCP's - especially CCP-EM & CCP-BioSim – Dave Brown to advise. Make sure we do not lose the crystallography focus!

Some of the points discussed

- MR focusing on difficult problems – keep the deep dive
- Tell people what they need to be doing rather than just examples
- Encourage use of techniques to obtain good crystals, or make the best of crystals
- Focus not just on a lot of techniques but when and why to use them!
- What would you want your student to be exposed to? Make them aware of variety of ways.
- Do we want to include XFEL? Don't exclude but not many people use it at present.
- Metals – Eleanor done a good paper regarding this recently.
- Question: should we have QC & proteins; this is probably a talk but not a session

7. CCP4 – news for publishing the virtual special issue, discussion (Ivo Tews, Lousie Jones, IUCr)

IT: Initially the special issue was meant to be educational, but it has to adhere to scientific publishing rules. Reviewing: authors may have to be dealing with “unreasonable requests”, or author may submit work unsuitable for scientific publication. However, we can use a variety of categories and formats such as reviewers and keep an eye on what category an article fits into.

LJ: Publication date now a week or so after acceptance date – online and live. We will therefore have a virtual special issue. There remains the need for a cut-off date. This means: build up over time under one issue as papers can be added when approved until the cut-off date. Bulk of publicity will be done after the cut-off date. The virtual issue can have a cover – winning illustration from the competition will go on the website.

Need to get the articles in quickly in order this to work best. Submissions would need to be in before Easter. We need to empower editors to be more “pushy”. Phoning people up can be more efficient than e-mails!

There is new template letter for contacting authors in order to remind them of their commitment. Each author will get a separate url to upload their article. Louise will contact authors with the relevant details. Organisers should encourage authors to come to the SW with manuscript.

Printed issue? Options: do we still want this? About half of the WG2 attendants voice they would like to have a hard copy as it is helpful for new starters/students. But there is cost for printed copies, and online has the advantage of online search. The final vote was for a virtual, online only issue, to be brought forward to Exec for ratification.

8. What's new in CCP4 (Kyle Stevenson, Ronan Keegan)

CCP4 Grant 2019-2024. New core team member Tarik Ronan Drevon to start in February under David Waterman working on Electron Diffraction.

Finalising release of 7.1 for all OS – few bugs at present. Pre-releases are available – contact core team if want to try the current version. Main content: Updates to many applications; CCP4i2 – new improved deposition task introduced plus other improvements; Gemmi – between Global Phasing & CCP4 – library for use in MX programs; DIALS/DUI - DIALS2 – now does scaling and merging sets, new spot finding algorithms and more robust.

The CCP4 cloud client is now available and runs jobs on clusters at RAL or can be installed locally. SIMBAD has been updated and can now use Phaser to test domain search models.

To do: Testing & fix minor bugs, prepare download pages.

9. Serial Crystallography (Ivo Tews)

ESRF EBS — extremely bright source — on time with their upgrade. We (the users) have to think what to with this new resource. Move out of your comfort zone! Crystallography is changing!

DIALS goes serial (Graeme Winter)

Flexible workflows for challenging data. Speed improvements, but not yet as fast as originally planned (10 years ago). Multi-crystal analysis. Fully Python 3 compatible. Xia2 looks the same to the use, running XDS / DIALS. Serial crystallography is already a standard application, but algorithms on refinement and integration of serial data are not so well defined and depend heavily on prediction. 2020+: make serial data processing friendly to non-technical users, including automation!

The serial crystallography experiment (Mike Hough)

Processing of serial crystallographic data is challenging — poorly defined and understood. Advantages to use the method: Ideal for room temperature, damage-free XFEL structures. I24: Fixed targets. A silicon chip-based system, user-friendly, but very non-automated — large beamline team needed. For good feedback — need a data-processing expert at the beamline.

Processing serial data - what's missing (Danny Axford)

“It's like synchrotron MX from the 2000s.” Top tips: Look at diffraction images; find and check log files; check all input is read; look at unit-cell distributions; run tests on small subsets of data; nothing runs automatically.

Dynamic crystallography BAG at Diamond (Danny Axford)

Travel grant for UK-based researchers.

Ivo: What tools would fit into CCP4? Danny: Linking programs into pipelines would be useful. Ivo: Scaling isn't really addressed. Graeme: Scaling is limited by the quality of the data.

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

Proposed date: proposal 20th May 2020. Location: London.

11. AOB

None.