

CCP4 WG1 Meeting 2024

3rd January 16:30-17:30

In-Person: Daniel Rigden, Eugene Krissinel, Dave Brown, Mads Gabrielsen, Arnaud Basle, Ed Lowe, Steve Prince, Randy Read, Vilmos Fulop, Briony Yorke, Arwen Pearson, Martin Walsh, Dave Hall, Alistair Siebert, Dave Stuart, Paul Rowland, Tom Burnley, Garib Murshudov, Ben Bax, Robert Oeffner, Elspeth Garman, Andrew Quigley, Mike Hough, Peter Moody, Stephen Carr, Ivan Campeotto, Jon Agirre, Ivo Tews.

Via Zoom: Keith Wilson, Kathryn Cowtan, John Helliwell, Pierre Rizkallah, Paula Salgado, Atlanta Cook, Richard Pickersgill, Jennifer Littlechild, Roberto Steiner, Johan Turkenburg.

1. Chair - Opening remarks: **Ivo Tews** 5 mins

Welcome. Definition of CCP4WG1 as the PIs in the UK doing crystallography and eligible to submit grants, plus technical support staff and industrial users (license holders) – this is a forum to steer CCP4 development.

The grant was submitted to the BBSRC. Challenges: selection of projects, but this also identified further good and fundable science (e.g. in ED and AI, the latter high on the UKRI agenda). Inflation has put some pressure on the planning, so we have submitted a 4 yrs plan within the £2m ceiling.

Challenges and opportunities for CCP4: Synergies with EM are to be further explored in the future as we are serving the structural biology community; at the moment, we are addressing CCP4/CCP4 inter-compatibility. Code forward porting of the suite and potential retiring software is to be looked at. ED&I is high on the agenda, and this directly concerns people and projects, exec membership, and CCP4 becoming more international.

Nomination for Briony Yorke (Leeds) to come onto Exec (proposer Ivo Tews, seconded Dave Hall).

2. Infrastructure – core team report: **Eugene Krissinel, Charles Ballard** 5 mins

EK We are at CCP4 v8.0 and with 16 updates over this and the last year. Preparations for update 17 are in progress to respond to changes in operating systems as smooth transition, does not include new applications. We are preparing to move development to the GitLab platform (gitlab.com).

CB Projects will (probably) fully migrate to GitLab by end of this year. It may take about a week to move across as this is not a complex operation (same engine). There is a test release of Coot 1.0; scripting is problematic at the moment.

3. Finance: **Charles Ballard** 5 mins

Year	2020-21	2021-22	2022-23	2023-24*
Main (£10.5k)	122 (+9)	136 (+16)	161 (+33)	167 (+19)
Subs (£7.55k)	43	49 (+1)	49 (+1)	50 (+1)
Ac (£3.5k)	2	2	2	5 (+3)

Total	167	187	212	222
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Moderate increase in licenses (19 gained, 11 lost).

Year	2020-21	2021-22	2022-23	2023-24*
Income	1,657 k	1,705 k	1,988 k	2,110 k
Expenditure	1,630 k	1,654 k	1,680 k	1,950 k
+/-	-138 k	-51 k	-308 k	-160 k

2022/23 saw a large underspend, £308k due to the increase in licenses, £300k+ allocated to year, staff turnover and delays in filling positions. NB as invoicing for external positions is by 3 months in arrears it typically takes 5-12 months for new posts to appear in the accounts.

2023/24 is predicted to again show an underspend, £160k. Part of this will be used in renewing aging computer equipment. With full retentions, predict small underspend for 2024/25.

Price increase in 2024/25 (first since 2018)

- £10,500 to £12,000 for main sites
- £7,550 to £8,000 for subsidiary sites

The pinch point in 2025/26 when several contracts are up for renewal (include large increases to cover recent inflation). CCP4 exec is asked to look at this and propose adjustments; presently discussed: £13,000 for main sites, £9,000 for subsidiary sites. Would WG1 approve this? Will come before WG1 again if proposed. Vote: Yes.

We run a proforma mechanism to invite scientific projects for funding.

4. CCP4 Current Grant: **Kathryn Cowtan**

5 mins

The grant has four work packages with variety of posts spanning different periods. WP1 from DLS/Cambridge investigated the relationship between data and refinement, with machine learning aspects. Release of ServalCat (next generation refinement software) was a major contribution not originally proposed that developed during the runtime of the grant. Several publications. WP2 from York delivered shift field refinement and hybrid model building. A lot of additional tools on model building were developed, machine learning was incorporated. There has also been developments on carbohydrates. Five publications. WP3 from Liverpool on use of contact prediction approaches in structure solution / validation underwent a major revision due to the advent of AlphaFold2 prediction. Produced six publications with two in preparation. WP4 initially was a bit blue-sky to investigate electron diffraction and was not predictable but was successful as it laid some groundwork to the very difficult problem and is proposed to be continued to working software solutions by further funding. Three substantial papers on the technique. There was also a work package on impact and dissemination that has seen revision of web pages and supported work of the working group 2 on revision of software

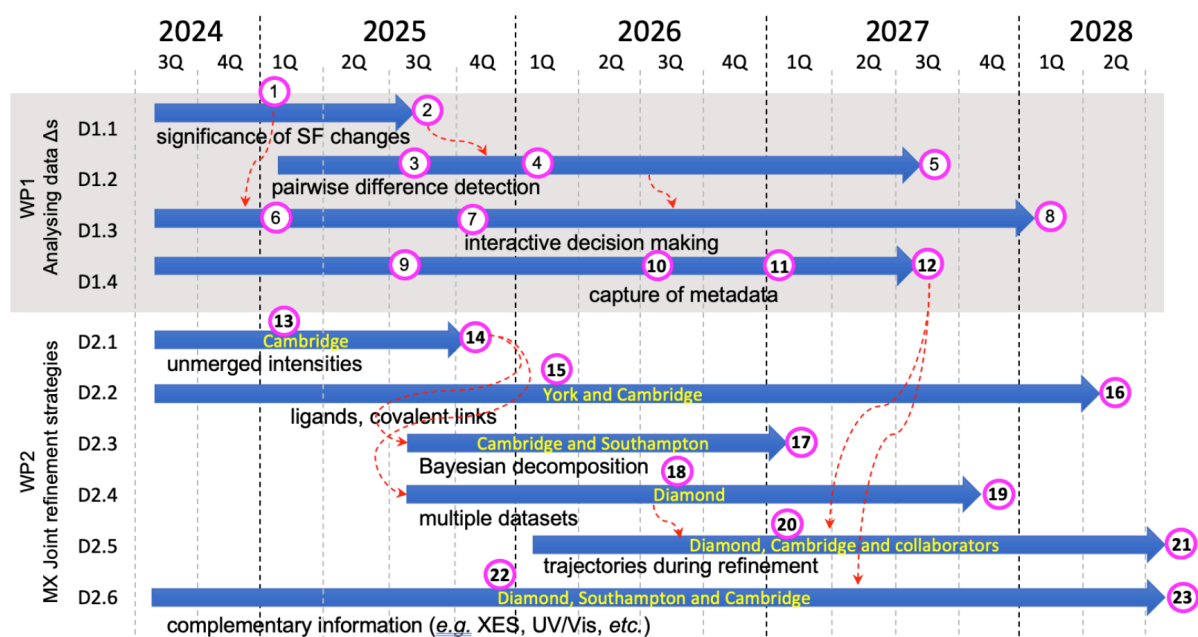
development and delivery of the annual study weekend. The entire network produced a range of papers, including the new general references for the CCP4 suite.

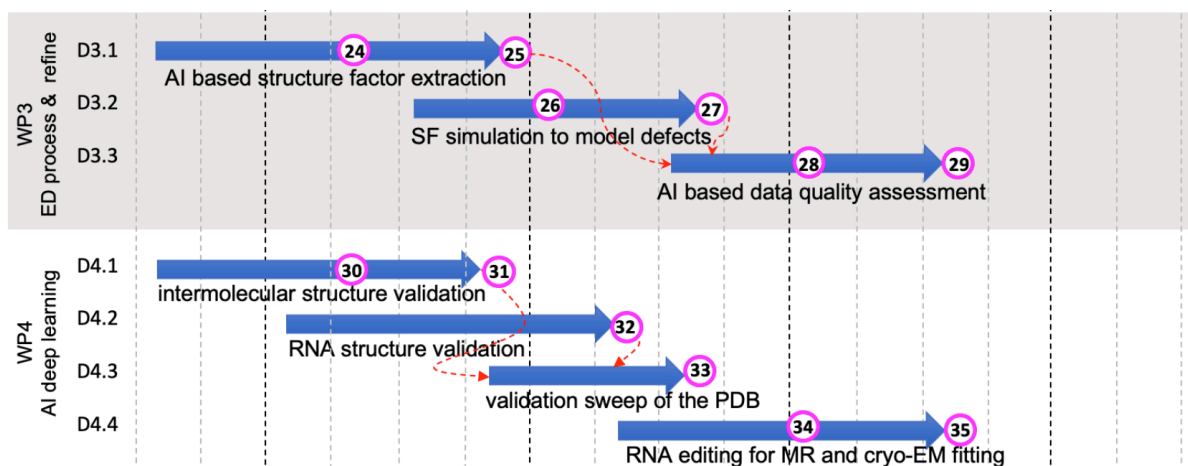
Please cite: Acta Cryst D79 (2023), 449-61.

5. New Grant Application: Ivo Tews

5 mins

We submitted the new grant proposal to the BBSRC last autumn; we had a meeting at Cosener's with the BBSRC to advise us. There were five reviewers to look at the grant, asked to scrutinise the work package, and their detailed comments were taken on board. The general comment was that this proposal is timely and meets challenges CCP4 should be expected to address. **WP1** A statistical framework for analysing structural change and its representation in data (time and/or state) (Hough, Evans, Winter; Diamond Light Source) **WP2** Joint refinement of related structures (Murshudov, Agirre, Tews Orville; Cambridge, York, Southampton, DLS) **WP3** Advance computational methods for data processing and structure solution to exploit advantages in ED (Krissinel, Waterman; Research Complex at Harwell) **WP4** Exploiting Deep Learning-based structural bioinformatics for crystallography (Rigden; Liverpool). Sections on governance and ED&I were included. We have a core team that distributes software to the users and insures the code base. We have WG2 and the developers meeting to be looking at and working on software. The CCP4 executive to which these groups and the grant holders report and to whom the user base inputs via WG1 steers the activities of CCP4. Diversity and inclusion is more than gender and we have a good, young and diverse contributor user base which should be fostered.





6. WG2 report: **Arnaud Basle, Jon Agirre**

5 mins

New chairs have been elected in 2023 (Arnaud Basle and Jon Agirre) and have held five meetings in 2023, one in person (London) and four on Zoom (2h each). This formula seems to work OK. New software was trialled: import_serial, Moorhen, DUI2, Servacat, new monomer library. The *Ligands interest group* met in November and will report at the upcoming WG2 meeting, dealing with PDB disposition.

7. ED&I activity: **Jon Agirre**

5 mins

Early Careers Researchers are a focus, as evidenced by the new general CCP4 paper that has 94 diverse authors – compare this to the earlier 2011 publication! We tried to be inclusive with this publication. Around 20% female, we see change. For meetings, a code of conduct is in place (all attendees accept this to attend). Pronouns are now used to be more inclusive.

The Equity, Diversity and Inclusion team lost Melanie Vollmer. Briony Yorke (Leeds) volunteered to join.

Ivo Tews proposes internationalisation of membership, first to be implemented (and thus discussed) at the CCP4 executive.

8. The CCP4 Study Weekend, Meetings & workshops: **Arnaud Basle, Jon Agirre** 15 mins

We need to discuss how the hybrid / streamed format is received (at WG2); we already discussed whether there should be a price tag on online participation and decided not to. Some of the meetings and workshops don't lend them to being hybrid. Lunch time bytes work better with small amount of people.

Workshops

- Sponsored events: SWSBC, Northern meeting, BCA summer school
- Full workshops: DLS (Nov 2023), APS (Mar 2023), SPring-8 (Nov 2023), SEACourt (Jan 2024)
- Short workshops: Dubrovnik (Apr 2023), Madrid (May 2023), Prague (May 2023), Oulu (May 2023), IUCr (Aug 2023)

Study weekend

- 2023's smaller hybrid event was surprisingly expensive, costing £124k, with income of £48k (220 in person, 300+ virtual).
- Registrations for 2024 in person is at 205, with 400+ virtual.

How do you want to organise the future? We organise the study weekend for 250 people to attend in person. It is noted that the CCP4 study weekend in the first week of January is awkward in timing for many.

Arwen Pearson: If you had meeting one week later you are into teaching and traffic.

Next Study Weekend. Previously we had a rota of topics, like data collection, phasing, molecular replacement, refinement, model building and validation. What would you like for 2025?

Keith Wilson: Validation is a good one, if we broaden the definition and extend to data validation.

Peter Moody asked is that big enough?

Dave Brown: We don't need to have a whole meeting on one thing. Validation is a good component, not the whole thing. We are structural biologists not just crystallographers.

Ivo Tews: So probably best to have a general meeting and include focussed sessions, such as validation or EM. WG2 to discuss.

9. AOB

CCP4 Exec: current list of members, nominations

Elected		Co-opted	
Ivo Tews	2023- Chair	Eugene Krissinel	Head core team, WP PI
Dave Brown	2023 - Industry	Kathryn Cowtan	Grant WP PI
Judit Debreczeni	2017-23 Industry	Garib Murshudov	Grant WP PI
(Mike Hough	2021-23)	Mike Hough	Grant WP PI
Helen Walden	2022-24	Dan Rigden	Grant WP PI
James Murray	2022-24	Gwyndaf Evans	DLS Rep
		Martyn Winn	STFC Rep
		Martin Noble	i2 lead
		Randy Read	
		Jon Agirre, Arnaud Basle	WG2 (Joint Chairs)
		Keith Wilson	Scientific manager