



# Agenda

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<b>Meeting title:</b>	CCP4 Working Group 2 meeting	
<b>Date:</b>	Wednesday 6 <sup>th</sup> June 2018	<b>Time:</b> 11:30 – 16.00
<b>Location:</b>	Francis Crick Institute, London (entry from St Pancras Station)	
<b>Circulation:</b>	ccp4wg2@stfc.ac.uk	
<b>Signed up:</b>	Svetlana Antonyuk, Charles Ballard, Eleanor Dodson (ED), Kaushik Hatti, Mike Hough, Ronan Keegan, Eugen Krissinel, Andrey Lebedev, Ed Lowe (EL), Airlie McCoy, Karen McIntyre, Rob Nicholls, Andrew Purkiss, Randy Read, Dan Rigden (DR), Mark Roe, Massimo Sammito (MS), Kyle Stevenson, Ivo Tews (IT), Isabel Usón (IU)	
<b>Apologies:</b>	Arnaud Basle, Dave Brown, Marc Morgan, Paul Rowland, Jose Trincao, Ville Uski, Melanie Vollmar, Pamela Williams, David Waterman, Keith Wilson	

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## *11:00-16:00 WG2 agenda*

Please arrive for coffee at 11:00.

## *11:30-16:00*

- Approval of minutes from the London The Birkbeck WG2 meeting 24/1/18
- Chairs report (Ivo Tews)
- CCP4 activities, workshops and courses (Ivo Tews, Charles Ballard)
- CCP4 SW2018 “Multi-Crystal and Data Collection”, proceedings (Charles Ballard)
- Proposed programme for the SW2019 “Molecular Replacement” (Isabel Usón, Randy Read, Ronan Keegan)
- Proposed Special Issue “Molecular Replacement” (Isabel Usón, Randy Read, Ronan Keegan)
- Open discussion – MR Study Weekend 2019 programme
- Talks: Molecular Replacement – new developments
  - a. Unconventional MR with AMPLE: recent developments and future prospects (Dan Rigden)
  - b. MRparse: a decision support system for MR (Dan Rigden)
  - c. MORDA (Andrey Lebedev)
  - d. Simbad and Contaminer (Ronan Keegan)
- BBSRC grant submission for continued funding of CCP4.
- 40 years of CCP4
- Web Page Launch
- Take note of the date of the next meeting (proposal 26<sup>th</sup> September or 3<sup>rd</sup> or 10<sup>th</sup> October 2018)
- AOB

# Minutes

## 1. Approval of minutes from the London WG2 meeting 24/1/18

The minutes from the London WG2 meeting 24/1/18 were approved.

## 2. Chairs report (Ivo Tews)

IT reported on presentations at the Cosener's Developers retreat and the EXEC meeting at this retreat. The "Pathway to Impact" for WG2 activities as part of the upcoming grant proposal was presented. The layout of the new CCP4 webpages was shown. At these meetings, a proposal for the route of software into the suite was proposed:

- New developments *should* have a software demo at WG2
- Developers must contact the core team to check compatibility of the software with the suite
- WG2 and core will then give a recommendation for inclusion
- The decision of inclusion lies with the CCP4-Exec

An alternate model is to understand the community needs and follow up with developments. This is happening through CCP4 workshops and it should apply to all new developments funded by CCP4. At WG2, we further discussed:

- that this/these pathway may not be widely known and should be publicised (e.g. on web pages)
- licensing issues: in general, licenses must follow the STFC-CCP4 license mode; however, inclusion of 3<sup>rd</sup> party software is possible in cases (example: ARPwARP)
- there should be a strong steer towards avoiding a crowding of the suite
- the transition from external software into the suite requires maintenance and support:
  - which depends on software writing style;
  - we need to be mindful that a substantial amount of time is required for maintenance of the software
  - inclusion of software written by others (rather than core) adds another layer of complexity (compare to the PHENIX model where software comes from a few)
- A testing environment is clearly needed:
  - DIALS team have some good testing protocols, learn from this?
  - new post should assist with this DIALS test/RR tests
  - maybe should drag in similar to augment our nightly builds/tests
  - some developers may have tests we could adapt
  - clearly, testing is a priority, but a test environment would ease use for developers
  - we minimally need to cover DIALS/Phaser/Refmac (non GUI)
  - GUI testing should be discussed at GUI2 & JScofe meetings
  - need to identify tools with insufficient testing
- Handover of software into the suite, past and present difficulties:
  - branch-off after release
  - reverse engineering to bridge time between releases.

## 3. CCP4 Core Group Activities (Charles Ballard)

The following were supported:

- January: CCP4 Study Weekend (UK) – conference organisers
- February: CCP4 workshop (Israel) – workshop organisers
- June APS/CCP4 school (USA) – workshop incl. data collection organisers
- July SWSBC meeting (UK) – conference sponsors/demonstration
- July: ACA 20018 – conference attendees with workshop/demonstration
- August: ECM – conference attendees with workshop/demonstration

- August: ECM computing school – workshop sponsors
- September: BCA Summer School (UK) – workshop tutors/sponsors, 30 attendees including one David Blow bursary student from Africa

Further plans:

- Northern Crystallographic Meeting (UK) is unlikely to happen; CCP4 would sponsor but lack of interested, to be brought forward to EXEC for further discussion (IT)
- Denmark (July) focussed on PHENIX, CCP4 presence?
- Brazil workshop – Action on Ronan Keegan
- New workshop in Thailand beginning of 2019
- December DLS workshop (UK) – workshop incl. data collection organisers
- December: AsCA conference
- Spring8 (Japan), RapiData (workshop) t.b.c.
- India workshop (late 2018)
- On-going: DLS BAG training (UK)

ED suggested that Core team could do 2 day workshops in the UK i.e. York, that could be short roadshow style to help students use the software. DR said we could also plan to do this when abroad. IU said some help with data etc. is also helpful, but workshops are needed to establish a common level of theoretical knowledge first. The DLS/CCP4 workshop was generally welcomed as good for both, new and more advanced users. MS suggested there might also be more emphasis in workshops on users to show how they are using the CCP4 suite.

#### **4. CCP4 SW2018 “Multi-Crystal and Data Collection”, proceedings (Charles Ballard)**

The proceedings are on track for the 2018 study weekend. Some authors need reminding of deadlines though and chasing. Action on the organisers.

#### **5. Proposed programme for the SW2019 “Molecular Replacement” (Isabel Usón, Randy Read, Ronan Keegan)**

The proposed program for the study weekend was shown and discussed. Six sessions were proposed:

- Session 1 – Introduction: MR Perspective, targets and Bioinformatics.
- Session 2 – Exploiting prior knowledge of protein structure
- Session 3 – Considerations on data and model preparation
- Session 4 – MR with fragments and combining information
- Session 5 – Model completion as an intrinsic part of MR
- Session 6 – Case Stories

The proposed speakers list includes 24 speakers, 11 of which are female. The lunch time bytes were proposed, and a novel session called “MR clinic” was proposed that should enable attendees to send in difficult cases prior to the meeting and discuss them there.

#### **6. Proposed Special Issue “Molecular Replacement” (Isabel Usón, Randy Read, Ronan Keegan)**

All invited speakers should be able to produce an article for the ActaD special issue “Molecular Replacement”.

#### **7. Open discussion – MR Study Weekend 2019 programme**

Gaps in the programme were pointed out to the organisers in Nucleic Acid structures. The programme was approved.

## 8. Talks: Molecular Replacement – New developments

- Unconventional MR with AMPLE: recent developments and future prospects (Dan Rigden)
- MRparse: a decision support system for MR (Dan Rigden)
- MORDA (Andrey Lebedev)
- Simbad and Contaminer (Ronan Keegan)
- Pipelines and online services (Ronan Keegan)

A discussion on pipelines included a consideration of selection and referencing of software.

## 9. BBSRC grant submission for continued funding of CCP4 (Ivo Tews)

Because of time constraints, this was only briefly reported on. The structure into work packages and the deliverables of the grant and a Gant chart were shown:

- Submitted through WG1 route (Dave Brown, Kent)
- WP1 diffraction (DLS/Evans and LMB/Murshudov)
- WP2 refinement and model building (York/Cowtan)
- WP3 molecular replacement to validation (Liverpool/Rigden)
- WP4 electron diffraction (STFC/Krissinel)

## 10. 40 years of CCP4 (Ivo Tews)

A central meeting in London aimed at demonstrating the significance of CCP4 as a project will take place in the Royal Society on 9<sup>th</sup> July 2019. A suggestion is a CCP4 '40<sup>th</sup> Jubilee' memory stick suggested. WG2 discussed the contents:

- Software: link only, to avoid software going out-of-date
- Teaching and tutorials
  - could be implemented on a Linux bootable partition with software, requires 8GB (EL)
  - may not boot on macs
- CCP4 special issues, Whats-New / Whats-Old (historic review)

Funding available to promote event further - IT open to suggestions on this point.

## 11. Web Page Launch (Eugene Krissinel, Ivo Tews)

IT presented a video demo of the new web page design. Open to CCP4WG2 in September for review.

## 12. Take note of the date of the next meeting.

Possible dates are 26<sup>th</sup> September or 3<sup>rd</sup> or 10<sup>th</sup> October 2018. Location: London.

## 13. AOB

None.