

WG1

January 11th 2018

Exec report and minutes of the WG1 meeting

09:00-10:30

1. Dave Brown (DGB) Thanks to

- Organisers of the 2018 Study weekend on **Multi and Serial Crystal Data Collection and Processing** in Nottingham UK, 10-12 Jan. 2018

Arwen Pearson (CFEL, Hamburg), Robin Owen (DLS, UK), Max Nano (ESRF, Grenoble), the organisers who put together a stimulating programme with an outstanding set of speakers. Core team and STFC funded staff for assistance in organising and running the meeting.

- Core team and CCP4 and funded staff in supporting integration, bugs fixes and distribution of the software suite.
- Keith for his management role and “oiling the wheels” of CCP4 and with Martin and the rest of the i2 team continued development of the interface.

Additionally, I would like to thank the non-directly funded developers who continue to provide enhancements to the suite and assisting in implementation of functionality into GUI2

DGB attended a joint CCP steering group meeting to promote cross-fertilisation and learning between the running CCPs – suggestion for a combined CCP4 CCP Bioinformatics meeting/workshop for 2018.

2. Finance (See additional document)

DGB: Finance looking healthy – increase in income this year of 14%. Considerable number of small drug discovery start-ups buying licences (esp. in USA and Asia).

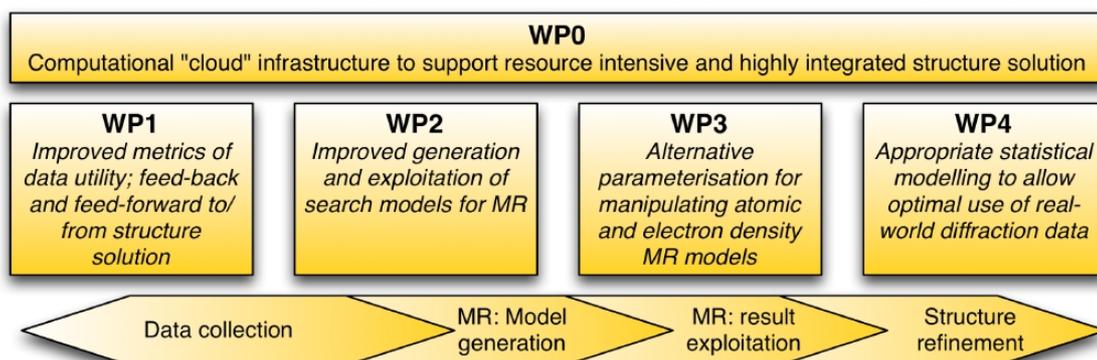
CCP4 are spending down excess by funding an additional post to support core activities as well as funding study weekend, sponsoring meetings with CCP4 presence and other workshops and training events.

Keith Wilson (KW): Workshops – comment that we do big workshops that consume a lot of core team time in India and Asia – do we do enough small institution visits and local training in Europe/UK. EK: would be extremely useful for i2 developers. IT: we already have regional meetings, some of which are very successful – targeted at students and postdocs (i.e. main user base) – that include software demos. Note: that the Northern (Carlisle) meeting attendance is going down – MN: notes there have been some issues with scheduling, could also be conflicts with people focusing more on EM. EK: need to organise more workshops at international conferences. ED: used to run a post study weekend 1 day workshop in York for the Indian SW visitors and this was very useful. Simon Newstead: Asking about whether there are geographical matches to hires/moves in terms of regional meeting attendance? KW: joint CCP-EM CCP4 meeting in the north – moved to Newcastle? Katy Brown: would like to see more attendance of CCP4 at the BCA/BSG meetings. DGB: lunchtime byte type activity is the thing we should be focusing on, always very popular. Thomas E: Leeds sending fewer people to

Carlisle, would be more interest in joint EM/MX meetings. Nick Keep: London structural biology meeting every 3 months, Martin Noble: same for northeast – could target these as workshop venues. DB: how much scope to add more CCP4 presence to the BAG trainings? Charles Ballard: already done.

DGB: Summary - appetite for localised workshops and for regional meetings that include more Structural Biology complementary methods (CCP EM, CCP BIOSYM, CCP NMR).

3 CCP4 Grant 04/2014-04/2019



WP Leads

WPO Eugene Krissinel (EK)

WP1 Gwyndaf Evans (GE)

WP2 Dan Rigden, Randy Read, (DR, RR)

WP3 Kevin Cowtan (KC)

WP4 Garib Murshudov (GM)

All work packages on track for key deliverables – as with any grant a few minor objectives have been changed or deprioritised. A significant number of papers have already been published with more to come in the final year.

New Software developments across the suite

LUNCHTIME BYTES key development activities WG1 members are encouraged to attend.

4 Grant Renewal

We propose to submit a new CCP Grant in 2018 to ensure continuity in scientific developments, as the existing grant ends April 2019. The Grant is focused on novel scientific software development to meet further develop crystallographic methods.

WP1	Optimal signal extraction from noisy scattering data	(GE/GM)
WP2	Hybrid structural modelling at low resolution	(KC)
WP3	Exploiting contact prediction for structural modelling	(DR)
WP4	Extending X-ray methodology to electron diffraction	(EK/DW) links to WP1

5 WG2 (Ivo Tews Presentation)

- Ivo Tews (IT) WG2 continues to be highly active and for 2018 there will be a continued focus on testing of new programmes – e.g. DIALS Gui, I2 interface and documentation including Web-based.

IT gave an update on WG2 role. Will be a renewal of the CCP4 webpages this year.

New software into the suite: 1) demo at WG2 2) recommendation from WG2 to Exec for the software to be included in the CCP4 suite (or not!). KW: notes that new software must have a plan for maintenance medium to long term.

DGB: Should WG2 be more representative of the UK community (currently meeting venues are London/RAL centric)

Discussion about whether we should be retiring some software – comments that this was done partly with i2. Note that the problem with leaving some of this old stuff in is that even if it is not supported people still ask questions about it on CCP4BB but core team are not in a position to answer. General feeling that it's worth keeping some of this code, but clearly marking it as unsupported.

Randy Read (RR): suggests an i2 button that triggers an email to the CCP4BB or to the relevant ccp4 support to ask for help. General feeling this would be a good thing, but need to make sure there is actually the infrastructure behind to answer the questions.

Arwen Pearson (AW): Suggest announcing WG2 meetings on ccp4bb shortly before the meeting to encourage "local" attendees to come and remind WG1 members that they might like to register for WG2.

Next WG2 meeting 24th January.

IT: has defined a list of Diamond BAG leads to contact them about WG2 meetings. Any updates to Ivo.

WG2 + next grant proposal: IT: Highlight WG2 activities in the pathways to impact and request some funding to support activities and outreach.

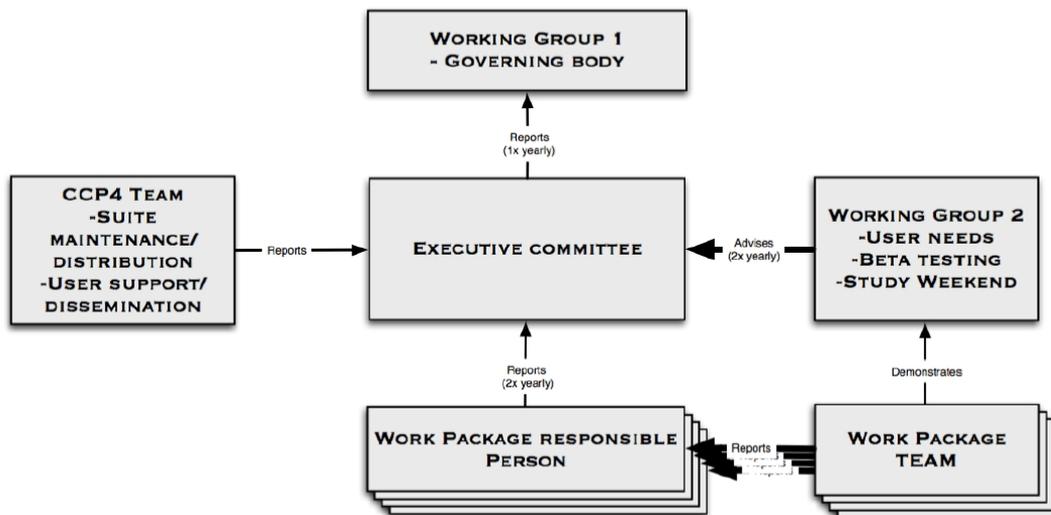
Suggestions for next year's SW:

- *Molecular replacement & model completion seemed a timely and well supported suggestion*
 - *Model prep*
 - *MR itself*
 - *MR of fragments*
 - *Model completion from MR*
 - *Co-variance*
 - *Low resolution MR*
 - *Use of models from non-crystallographic techniques*
- *General Phasing (last in 2015 with Experimental Phasing)*

Suggestions for organisers to Ivo before the 24th January.

6 Infrastructure

- GUI2 and Ligands/Validation key additional projects



At this years January Exec meeting and for purposes of the new Grant submission it was agreed to investigate the concept of introducing a SAC that may meet once a year or every two years to independently input into the progress on the grant but also feedback on the CCP4 Suite and scientific direction.

Request for comments on the ideas about an international advisory committee to advise Exec – primarily on the grant, but also on general CCP4 activities. Supported by a show of hands. Please send name suggestions to KW and DGB.

7 Current CCP4 Executive

We are looking for people to stand for CCP4 exec over the next two years please let Dave and Keith know if you are interested.

We have a couple of nominations for election by WG1.

Elected		Co-opted	
Dave Brown	Chair 2015 – 21	Eugene Krissinel	Head core team WP PI
Judit Debreczeni	2017-19 Industry Rep	Kevin Cowtan	Grant WP PI
Ehmke Pohl	2016-18	Garib Murshudov	Grant WP PI
Paula Salgado	2017-19	Gwyndaf Evans	Grant WP PI, Diamond Rep
Roberto Steiner	2017-19	Martyn Winn	STFC Rep
		Dan Rigden	Grant WP PI
Keith Wilson	Scientific manager		
Ivo Tews	Chair WG2	Eleanor Dodson	
		Randy Read	
		Phil Evans	

DGB proposed, Elspeth Garman (EG) seconded: Nick Keep to come on Exec in 2019 – voted in unanimously.

DGB proposed, EG seconded: Atlanta Cook nominated to come on in 2018. Voted in unanimously.

KW asked WG1 for endorsement of extending DGB as Chair of CCP4 Exec to 2021. Approved unanimously.

8 A.O.B

CCP4's 40th Birthday in 2019 – suggested celebration activities

- *at study weekend 2019 instead of “what’s new” to have a historical overview.*
- *½ day meeting in London at Royal Society with the great and the good. Inviting government and public officials. June 2019 is planned date (week after science week) – meeting with RS in the coming weeks to negotiate terms.*

RR: Acta Cryst D has been dropping in terms of both submissions and impact factor. Currently IF ~5 and 6 submissions a month. Please consider submitting to Acta D.

KB: Please try and support BCA/BSG. Note bursary's available for students to attend non-BCA meetings.