

CCP4 WG1 Meeting 2022

Zoom: 10th January 13:30-15:30

41 Dave Brown , Eugene Krissinel , Charles Ballard, Leo Brady Airlie McCoy, Atlanta Cook, Colin Levy, Dave Hall, Dave Lawson, Dave Stuart, Elspeth Garman, Frank von Delft, Gwyndaf Evans, Johnathan Grimes Ivo Tews, James Murray, Jennifer Littlechild, Johan Turkenburg, John Heliwell, Judit Dubreczeni, Keith Wilson, Kevin Cowtan, Mark Roe, Mark Sanderson Martin Walsh, Martin Noble, Mike Hough, Nick Keep, Paula Selgado, Peter Moody, Pierre Rizkallah, Randy Read, Ronan Keegan, Richard Pickersgill, Sheikh Mohammed Arif, Snezna Djordjevic, Steve Prince, Svetlana Antonyuk, Vilmos Fulop, Martyn Winn, Yvonne Jones

1. Chair: Opening remarks 13:30

This year has been another COVID affected year and I would like to take the opportunity to thank all those involved in CCP4, The Core team, developers and CCP funded positions and STFC support staff and the Executive committee as well as active WG1 and WG2 members (which will be mentioned later by Ivo) for all their continued commitment and engagement.

Apart from the obvious changes in ways of working driven by COVID we are also faced with a changing landscape within structural biology with the emergence of CryoEM and more recently the development of Alphafold which provides most of our users and developers new opportunities to support and drive the structural biology field forward.

CCP4 has always been about open collaboration to enable scientists to deliver crystallographic information to understand structural biology and these tools enable us to help experimenters focus on their scientific problems and we look at ways to integrate these methods into our workflows.

I would like to personally thank the organisers of last weeks study weekend (Melanie Volmar Rob Nichols and Svetlana Antonyuk) which certainly helped highlight the way in which we are already embracing these changes as a community

2. Finance: Charles Ballard 13:40

Moderate increase in license income – new licenses shows continued usage of crystallography
Reduced spend due to Study Weekend and a lot of virtual meetings as opposed

Spend down was suspended in the first year of COVID and we are pushing this out for next finance allowing.

3. CCP4 Grant: Kevin Cowtan

13:45

Thanked the study weekend organisers and highlighted that the exciting agenda reflected the way in which we as a community are embracing the changes in EM and Alphafold.

Highlighted a lot of outputs from the 4 work packages already in terms of publication and Workshops and working groups

WP2 Shift field method adapted for EM and Map refinement (as opposed to just models)
New stereochemical regularisation libraries are done (4 papers)

WP3 Contact MapPredictions

Most impacted by alphafold

Work with PISA to produce (2 papers to date 2 more in progress this year)

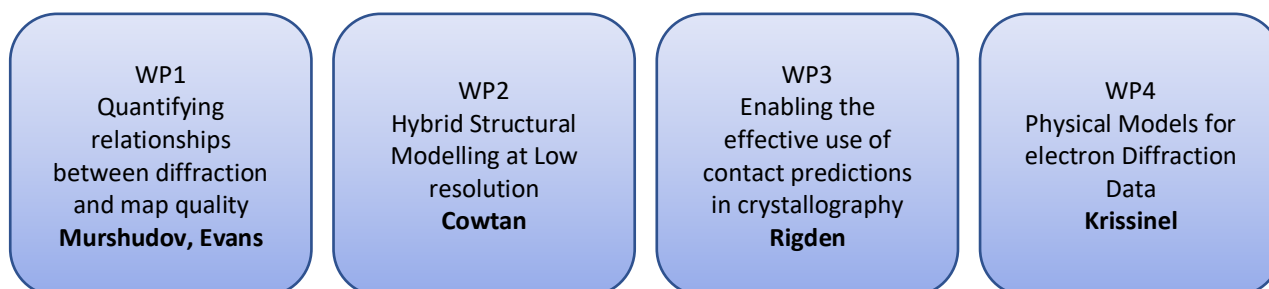
WP4 Physical Model for electron diffraction

Completed comparison of near Bragg approach to multislice and adapted DIALS and FELIX to develop and implement

IMPACT Ivo has focussed a lot of activity in ED&I team , starting CCP4 Documentation (Maria Fando) increased WG2 activity

Next Grant discussion We should have an outline of the proposal for the next Grant at the next WG1

4 Work packages over 5 years



Summaries of each WP

Outreach activities and Impact: Ivo Tews

4. Impact of AlphaFold2 on CCP4: Dave Brown, Dan Rigden and Ronan Keegan

14:00

MR pipelines and Validation

MR pipelines already coupled to EBI DB (AFDB) which will also include UNIREF90
MRparse updated to link and visualise sequence id and models in AFDB – already linked
into cloud and taking pLDDT scores linked. Ronan and Stuart have linked AFDV to
MrBUMP and CCP4mg. and Filo has rapidly picked up i=on using contact/distance
predictions for contact maps from RosettaFOLD and Alphafold2 to validate structures and
Machine learning approach in both Conkit and Iris (which will be in 8.0) which helps look at
things such as register errors.

Should CCP4 have its own AF2 (or OPENFOLD) service 5Villi has been looking into this)

Should CCP4 copy PHENIX to use Alphafold to build and refine and iterate between AF and
refinement to create better models/fit to maps

IT whats the advantage of our own AF install (makes it easy for users or interfaces to Colab)

RR Bioarchive PHENIX implementation is all in CCTBX so Open, the re-refine will be in
COLABfold notebook)

JD AF vs Openfold how many industrial users have AF license Dave suggested that currently
not many of the license holders will.

Ronan gave a quick DEMO on usage and access to AF DB at the EBI to resolve recent SAD
phased structure in both I2 and the CCP4 cloud.

Use of Phmmer API to access EBI AFDB – available to industrial License users.

5. WG2 report: Ivo Tews 14:20

Helps organise SW and Now 5 WG2 meetings often 40+ attendees and growing with
scientific focus

6. SW 2022 Report. Ivo Tews 14:25

1088 registered 689 students, 399 Researchers

Longer breaks and opportunity to meet was missed (not surprising given on-line meeting)
Hybrid is here to stay – more people and more diversity in attendees – more inclusivity-
talk lengths and diversity in speakers.

7. SW 2023 Proposals. Ivo Tews 14:30

8. WG1 need to suggest topics for next Study Weekend please put in the chat

James Murray Deep learning and structure prediction

Dave Brown How we use structures??

Judit D Machine/Deep learning But including Crystallisation Data processing structure
solution and modelling

Kevin Cowtan Structural Data for downstream users

Martyn Winn General Overview

9. Infrastructure – core team report: Eugene Krissinel 14:55

Showed cross Matrix of people and Main activities

Release and Updates – 18 updates for CCP4 7.1 now major focus on Release 8.0

Development and Collaboration

MR Alphafold , rewriting python codes, preliminary research into AI methods for data analysis and Quantum Computing and WP4 (Granted conformational landscape with EBI)

Python 2 to 3 and QT4 to 5

CCP4 cloud Framework for 3rd Party customised setups at a number of sites.

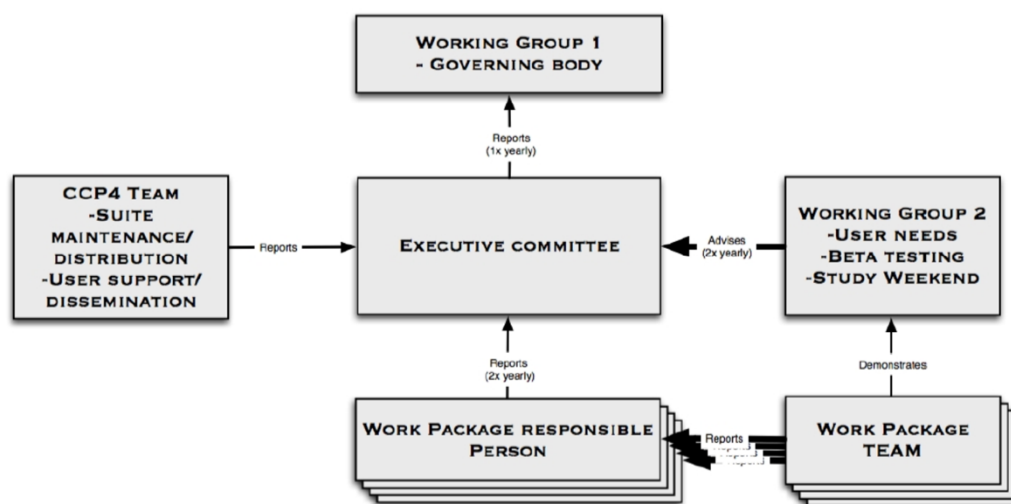
WebServices – still actively used 8000 big jobs from several hundred users still supported by STFC IRIS project

Documentation I2 documentation now all in RST format , Cloud documentation a little behind but project approved to improve this. Cloud now used in a number of teaching workshops

Outreach slowed

Virtu SA, Chicago, Motevideo and DLS

Also contributed to non CCP4 workshops Rapiddata, MX Oulu Finland, SWSBC



10. CCP4 Release Plans 8.0: Charles Ballard

15:10

Testing update manager and first cut release just about done (Findmy sequence and ML extend won't be on first release) Go to WG2 for friendly test release (Tarball and copy coot) Release End Feb Python 3.9 and QT 6 version targeted at end of the year.

KW acknowledged the big effort 5stuart , Ville and Oleg) for upgrade to Python 3 no more feature will go into 7.1

11. CCP4 Exec: current list of members

15:20

Elected	Co-opted
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Dave Brown	Chair 2015 – 22	Eugene Krissinel	Head core team WP PI
Judit Debreczeni	2017-23 Industry Rep	Kevin Cowtan	Grant WP PI
Nick Keep.	2019-21	Garib Murshudov	Grant WP PI
Mike Hough	2020-22	Gwyndaf Evans	Grant WP PI, Diamond Rep
Atlanta Cook	2019-21	Martyn Winn	STFC Rep
Dave Lawson	2021-23	Dan Rigden	Grant WP PI
Helen Walden	2022-24	Martin Noble	i2 lead
James Murray	2022-24	Randy Read	
		Keith Wilson	Scientific manager

12. AOB

15:25

Ivo Tews WG1 Numbers how do we publicise the meeting better to get wider representation of the community at WG1 - - Feel free to forward invites to other interested PIs...