

WG1 Minutes

January 9th 2019 Gallery 1 in EMCC

09:00-10:30

1. Chair: Opening Remarks

The current BBSRC grant for CCP4 runs until March 2019. A funding proposal for continued support of scientific developments within CCP4 for 5 years was submitted in April 2018 and was successful. This new Grant will commence April 2019 with Dave Brown as PI and COIs at Liverpool (Rigden), DIAMOND (Evans), RCaH (Krissinel), LMB (Murshudov) York (Cowtan) and Southampton (Tews)

Continued Development of (CCP4Cloud) cloud-based access to CCP4 software via CCP4-DAAS services utilising OpenStack. The CCP4-Online web services (<http://www.ccp4.ac.uk/ccp4online>) have been linked to ARP/wARP and PDB_REDO web services thanks to WestLife developments. This includes Single-Sign-On via ARIA authentication. The development of CCP4 Web Applications (jsCoFE) for remote crystallographic computations has progressed to a pre-release state, and the system was tested at 4 CCP4 international workshops. The system has been well received by test users.

Joint CCP steering pane looking for synergies see CCPEM obvious link and close collaboration – attend developers meeting at Cosener's but also CCP-NMR and CCPBiosymm.

Last year's 2018 Study Weekend was held at Nottingham on 10-12 Jan 2018 well received "Multi and Serial Crystal Data Collection and Processing" covering diffraction data collection at synchrotrons, FELs and on electron microscopes

Training schools in this period included of particular note: 1st CCP4/BGU Crystallography Workshop, Ben-Gurion University, Israel, 18-23 Feb 2018, APS, Chicago 18-25 June 2018; BCA-CCP4 Summer School at Diamond in August; India in October; Brazil in 14-24th November We organised a joint meeting with the BCA Industrial Group, 13–14th November in Durham, around the theme of NMR Crystallography, December – week long workshop

Key role due to the widening user base – less experienced more naïve users.

Highlights success and ease of use of the software but puts greater reliance on automatic methods and error checking and validation prior to PDB upload.

Revamp of the website near completion.

Additional Comments:

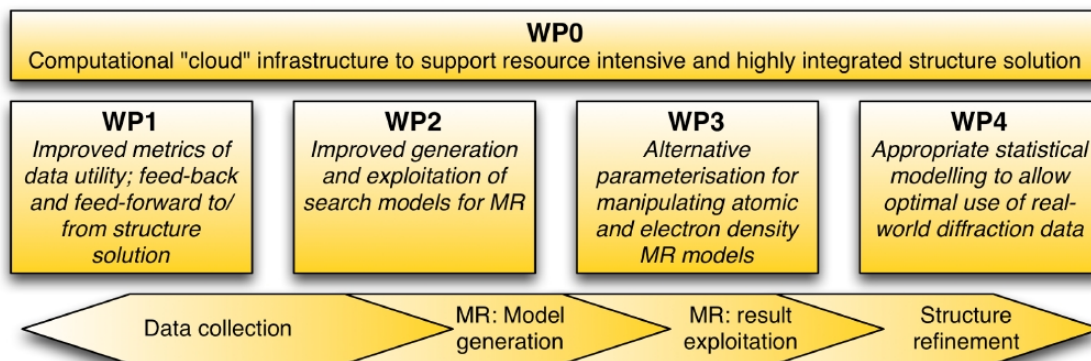
1. CCP4 is science driven, so is the recent grant application
Joint CCP steering group meetings – we highlight close links with CCPEM, developers cross-fertilisation by attendance to developers meeting maybe additional links with CCPBIOSIM

2. Finance (See additional document)

1. Income (Charles Ballard)
Slight loss in income
Government accounting rules changed, but this is being monitored/addressed

DB: 1m surplus/carry over, KSW: plans in place to spend approved by Exec
 Licence fee discussion; years warning required to licensees, financial planning 2 years ahead
 no plans to increase this year but may request increase to WG1 at SW2020

3. CCP4 Grant 04/2014-04/2019



WP Leads

WP0 Eugene Krissinel

WP1 Gwyndaf Evens

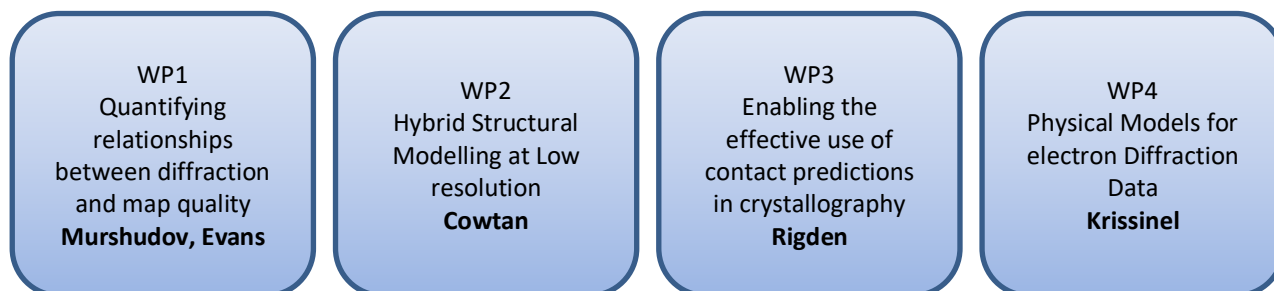
WP2 Dan Rigden, Randy Read,

WP3 Kevin Cowtan

WP4 Garib Murshodov

4. Grant Renewal. 2019-2024

4 Work packages over 5 years



WP1. Quantifying relationships between diffraction and map quality. (Evans, DIAMOND and Murshudov, LMB Cambridge)

Objectives:

To expand METRIX database and develop machine learning to support interactive decision through use data-quality as indicators of data-utility in structure determination.

To develop Fourier optics based relationship between diffraction, phase and map quality applicable to scattering experiments including X-ray diffraction, electron diffraction and also cryoEM. To develop new tools for refinement for electron diffraction data.

WP2. Develop shift field refinement methods for Hybrid Structural modelling at low resolution and provide significant refinement speed enhancements. (Cowtan, York)

Objectives:

To generalise and optimise shift field methods for wider applicability against multiple data sources.
 To implement new resolution independent model building framework in BUCCANEER and NAUTILUS
 To develop new stereochemical regularisation software library to enable critical speed improvements. To implement contact predictions developed in WP3 within BUCCANEER and NAUTILUS.

WP3. Implementation and exploitation of contact prediction approaches in crystallographic structure solution and validation. (Rigden, Liverpool)

Objectives:

To implement contact prediction methods in ConKit to accurately define domain boundaries for both protein construct design and model building.

To use contact predictions to provide a new size range of search models for Molecular Replacement.

To develop tools that utilise contact prediction to assist in validation and interpretation of macromolecular structures particularly identification of biologically relevant protein:protein interfaces.

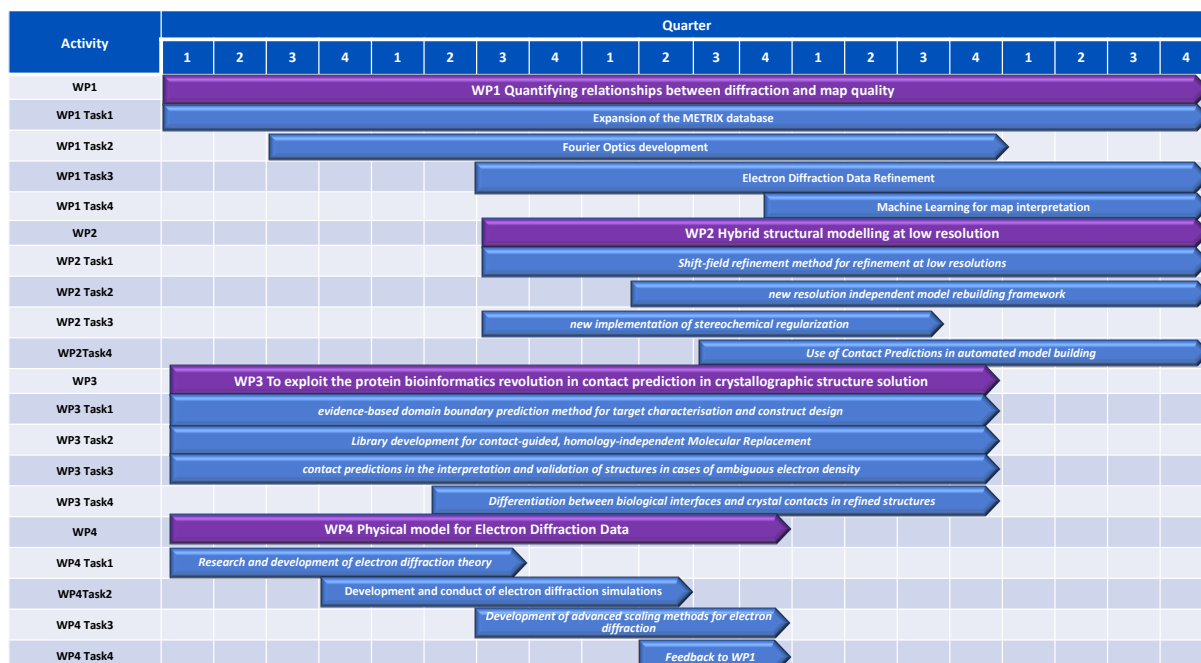
WP4. Physical Model for Electron Diffraction (Krissinel, RcaH)

Objectives

To develop a model of electron scattering for computer simulations to assist in software and experimental design.

To develop and implement scaling algorithms for electron diffraction

To link to WP1 to develop new tools for refinement for electron diffraction data.



Additional Outreach activities also funded– Role of WG2 and Meeting and workshop activities

Additional Comments/Observations

Funding goes to funding scientists

Dave Brown: speak to grant WP leaders if you have additional suggestions/synergies with your research or key general crystallographic issues or questions that require software development

Outreach in new approved grant WG2 is directly funded, attend and input

5. WG2 Update (Ivo Tews)

Discussion/Comments:

WG2 suggestion for SW this one MR 335 attendees

Shortlist for 2020: Low Res, Build and refine; Model building including auto; EM what is the X-ray component

Crystallographic methods should be key focus of the meeting

Elsbeth Garman later time means some overseas can't now tag onto Christmas visit

Martin Noble unlikely to be the topic or program that has resulted in lower numbers

Topics themes linked to grant

Gerard Bricogne remote attendees – check on follow on

Paula Salgado hybrid - model building in low res KW and PM model building where people spend their time Gerard Bricogne interplay X-tallography and EM

KB multi discipline projects coordinating efforts at Diamond /Isis Integrated methods Martin Noble suggested a day relating to low res and EM a least one session but high res and model completion. Peter Moody, Validation limits of interpretability

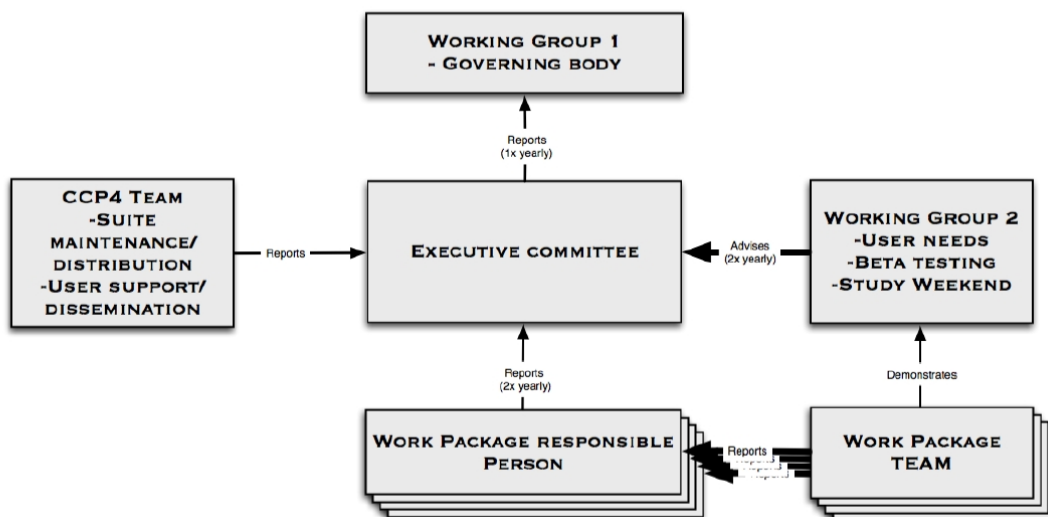
Ivo Tews please email additional ideas or names of people 23rd Jan London next WG2

6. Infrastructure

- GUI2 and CCP cloud

Key Comments:

All new developments go into i2 (not i1) Request to all PI's – please move forward with the times and encourage new and old staff alike to use i2. All training and workshop material is now in i2.



7. Current CCP4 Executive

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
Nick Keep	2019-21	Garib Murshudov	Grant WP PI
Paula Salgado	2017-19	Gwyndaf Evans	Grant WP PI, Diamond Rep
Roberto Steiner	2017-19	Martyn Winn	STFC Rep
Atlanta Cook	2019-21	Dan Rigden	Grant WP PI
Keith Wilson	Scientific manager		
Ivo Tews	Chair WG2	Eleanor Dodson	
		Randy Read	
		Phil Evans	

CCP4 Chair is also a member of the CCP Steering Panel that brings together all CCPs to share progress and look for synergistic opportunities. http://www.ccp.ac.uk/steering_panel.html

Open to Suggestion of new members

Paula Salgado, Judit Debreczeni started late, can they extend for one year?, end of 2020 - approved

Mike Hough elected to Exec, starting this year

8. 40th Birthday

We plan to hold a small meeting at the Royal Society on July 9th to celebrate 40 years of CCP4

Additional Comments:

Small meeting at the Royal Society

Submissions from first authors to see the spread of CCP4-use

Elspeth Garman: maybe young developers as well

Keith Wilson: young industrialists?

DaveBrown: prize, funds for travel to the meeting? To be approved by exec

9. AOB

Elspeth Garman: CCP4/BCA summer school, since 1990, looking for South location please contact Elspeth if any interest

Keith Wilson: commented Carlisle meeting disappeared. Suggested Alternative: York / Newcastle

Martin Noble: why did the last meeting disappear? Time limited?

Arnaud Basle: find a "central" place in the North.