

WG1
Friday January 8th 2022
Zoom Meeting

<https://ukri.zoom.us/j/97846794185>

10:00-11:30

Attendees 32 Participants

1. Chair: Opening Remarks 10 mins

After what has obviously been a difficult year for everybody, I would like to acknowledge the continued hard work and engagement by all personnel involved in supporting and developing the CCP4 suite and training related activities.

This year has seen the roll out of CCP4 7.1 with automatic updates for i2 and for the first time not providing an icon for i1 update to encourage additional transition to i2. This has highlighted that probably half of our users are still using i1. I encourage again people to move to a more object oriented environment utilised in i2 and cloud versions (as opposed to a file format in i1)

I would also like to thank the scientific organisers Atlanta Cook, Tassos Perrakis and Dan Rigden in arranging the first all on line CCP4 SW with over 1800 registrants/attendees as well as thanks for the support they have had from STFC CCP4 administration, WG2 and developers contributing with on line interactive sessions for the usual lunch time bites.

2. Finance (See additional document) (Charles Ballard) 15 mins

Charles gave a summary 1.5 million income stable major issue is inability to hut spend down due to the inability to attend/run a number of planned workshops. We have requested that we can defer the spenddown due to exceptional COVID circumstances

Precise budget is unknown

Keith commented we cannot fill posts easily

We brought forward hardware spend and replacing old hardware and

3. CCP4 Grant update April 2019-March 2024 (Kevin Cowtan) 25 mins

4 Work packages over 5 years

Kevin presented Gwyndaf update

WP2 Kevin gave an update. His WP has just started Paul Bind started Dec20 on shift field refinement

Shift fiels implemented and released in MR, model building pipeline

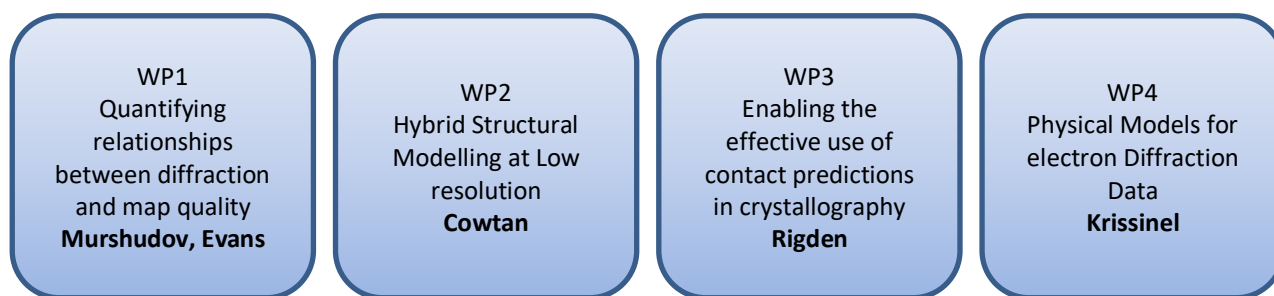
Pseudo regularisation developed implemented and released

A number of deliverables including sheetbend and SW papers published

WP3 Contact Prediction from Liverpool Javier Burgos-Marmó report will be in the minutes

WP4 Physical Model for electron Diffraction _ complexities of multiple scattering

Tarik Drevon has started in Feb 20



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

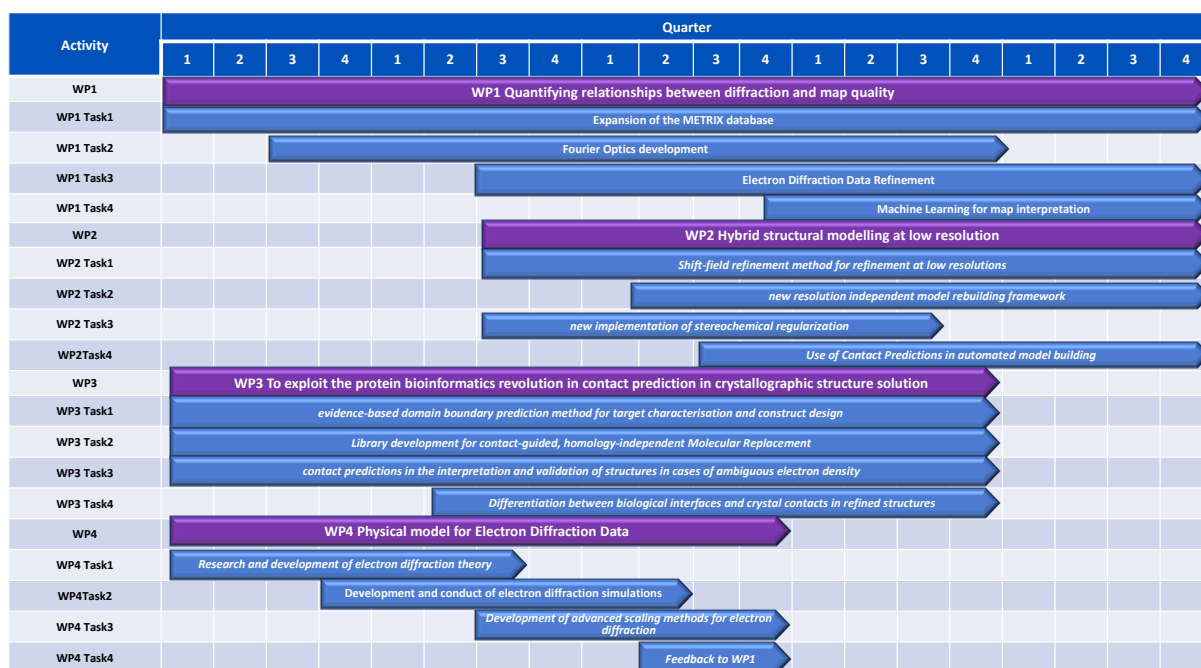
WP4. Physical Model for Electron Diffraction (Krissinel, RcaH)

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

Discussion on alpha fold John McGeeghan there was some discussion in the meeting

4. WG2 and SW Update (Ivo Tews) 20 mins

SW registration and attendance some useful starts in terms of monitoring attendance numbers

WG2

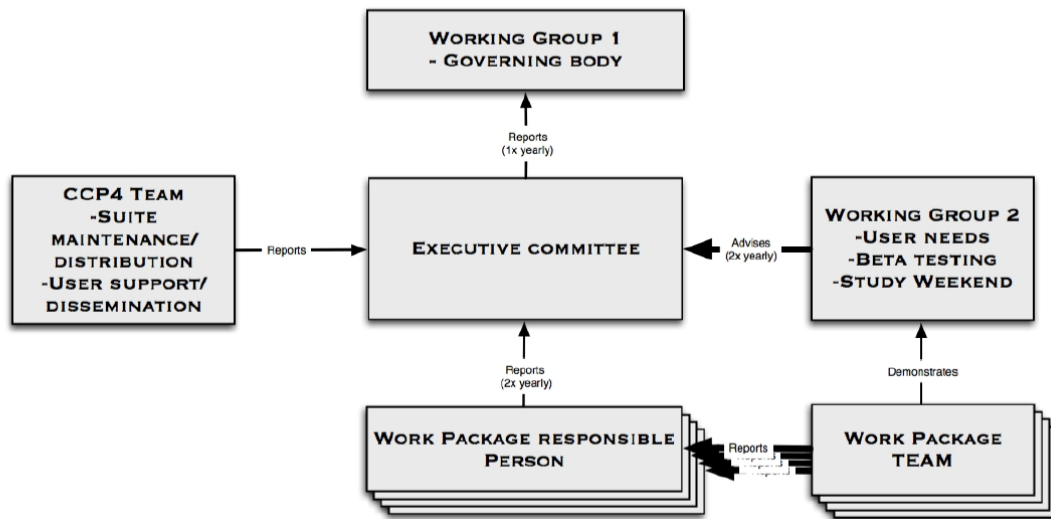
5. Current CCP4 Executive 5 mins

Elected		Co-opted	
Dave Brown	Chair 2015 – 22	Eugene Krissinel	Head core team WP PI
Judit Debreczeni	2017-21 Industry Rep	Kevin Cowtan	Grant WP PI
Nick Keep.	2019-21	Garib Murshudov	Grant WP PI
Paula Salgado	2017-21	Gwyndaf Evans	Grant WP PI, Diamond Rep
Mike Hough	2020-23	Martyn Winn	STFC Rep
Atlanta Cook	2019-22	Dan Rigden	Grant WP PI
Dave Lawson	2020-23	Martin Noble	i2 project leader
Helen Warden	2021-24	Randy Read	Phaser
James Murray	2021-24	Keith Wilson	Scientific manager
		Ivo Tews	Chair WG2

Transitions March Exec Meeting.

*New Industrial Rep Members for election this year.

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



6. AOB