

Chair's report to WG1

January 8th 2015

1 Thanks

As Chair and on behalf of the CCP4 Exec and WG1 I would like to personally thank the organisers of the 2015 Study weekend Airlie McCoy and Thomas Schneider. They have compiled a stimulating programme with an outstanding set of speakers.

I would like to acknowledge the hard work of the Core team and CCP4 funded staff in supporting integration, bugs fixes and distribution of the software suite.

Especially I would like to thank Keith for his management role and "oiling the wheels" of CCP4 as well as the transition support from the previous Chair Martin Noble.

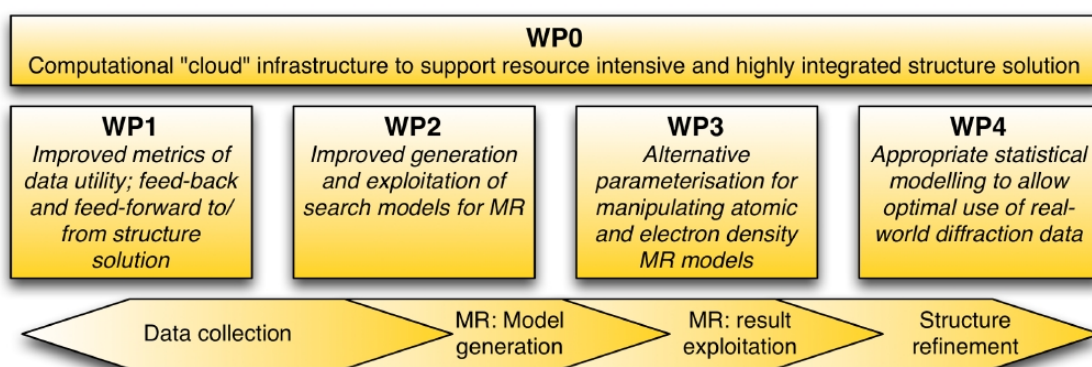
Additionally I would like to thank the non-directly funded developers who continue to provide enhancements to the suite and assisting in implementation of functionality into GUI2

2 Finance

The attached (and circulated) financial summary details CCP4's current and projected spend until the end of the current grant and based on the assumption of current head count being maintained. Our continued grant success and Industrial income have allowed the Exec to suggest no increase in Industrial fees for which we seek WG1 endorsement. Plans are in place to augment resourcing on GUI2 which will draw down on surplus that is currently projected. Thanks to Charles Ballard for maintaining details and providing CCP4 financials.

3 CCP4 Grant

All positions requested in the current grant have been staffed or individuals identified and posts accepted for 2015 starts.



The continued success of the streamlined build, test and distribution and easy implementation of upgrades by users has allowed the inclusion of the new GUI2 in the build in new releases which is accessible by invitation during the test/early roll-out phase.

4 GUI2

There has been major progress with GUI2 which now contains the majority of crystallographic capabilities thanks primarily to the efforts of Liz Potterton, Martin Noble with significant contributions from Phil Evans, Airlie McCoy, Jon Agirre, Kevin Cowtan, Rob Nicholls, Pavol Skuback and Raj Pannu. As already mention during 2014 Andrey Lebedev and Marcin Wojdyr created a CCP46.4.5 release which includes GUI2 and a significantly enhanced rapid update system together with a bug tracker. Until now most efforts and usage have focussed on Newcastle and York as test centres. A major focus for 2015 is delivery and roll out of GUI2 for which a steering and management group has been established, with Martin Noble as Scientific Lead and Keith Wilson as project manager reporting back to Exec. I would especially like to thank Liz and Martin for their continued efforts on GUI2.

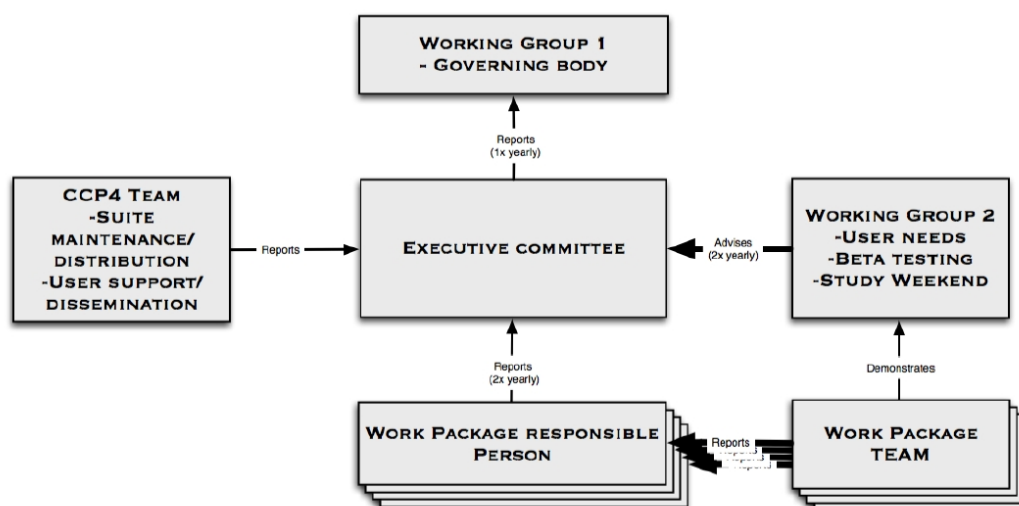
GUI2, together with ligands will be a major focus of the Cosener's Annual CCP4 review and developers meeting 24-26th March 2015

5 WG2

Ivo Tews accepted the role as Chair of WG2 in 2014 and has rejuvenated its activities. If you or researchers in your laboratory would like to get more involved with WG2 please contact Ivo.

6 Infrastructure

We have implemented the new reporting structure as highlighted in the Grant and included GUI2 as discussed earlier as a specific work package project and major focus for deliverables in 2015. Ligands also have a specific themed group which has led to the delivery of ACEDRUG.



This year the short reports of individual's activities will be provided for the March Cosener's meeting. For information on key activities WG1 members are encouraged to attend the Lunchtime byte sessions of the study weekend which covers recent developments and enhanced suite functionality.

Current CCP4 Executive

There are currently no representatives or executive roles due for election by WG1.

Elected	Co-Opted/Ex Officio
David Brown Chair 2014-2019	Gwyndaf Evans (DLS rep)
Ben Bax (Industrial Rep) 2014	Phil Evans
Frank von Delft 2013	Eleanor Dodson
Arwen Pearson 2014	Garib Murshudov
Elspeth Garman 2014	Kevin Cowtan
Ivo Tews 2014 (Chair WG2) 2014	Randy Read
	Martyn Winn (STFC representative)
	Eugene Krissinel (CCP4 Core Lead)
	Keith Wilson (Ex officio Scientific Coordinator)