Chair's report to WG1, January 4th 2014.

1 Progress in respect of resolutions from the last WG1 meeting

1.1 Discussion and vote: Thanks to meeting organisers

The 2012 study weekend was organised by Helen Walden and Pietro Roversi and covered the ever-young topic of Molecular Replacements. As ever, the blend of background learning and cutting-edge developments was stimulating for both regular attendees and newcomers to the CCP4-fold.
This year, we will be learning about the use of complementary methods through an excellent program assembled by Jon Cooper and Ivo Tews. It is customary for us to note our appreciation of the organisers of these meetings.

1.2 Election of a chairperson to take up office in 2014

An e-mail ballot of WG1 resulted in the election of Prof. Dave Brown (University of Kent) to the chairmanship of WG1 and the executive committee, with overwhelming support.

1.3 Discussion: portfolio of priority projects within CCP4

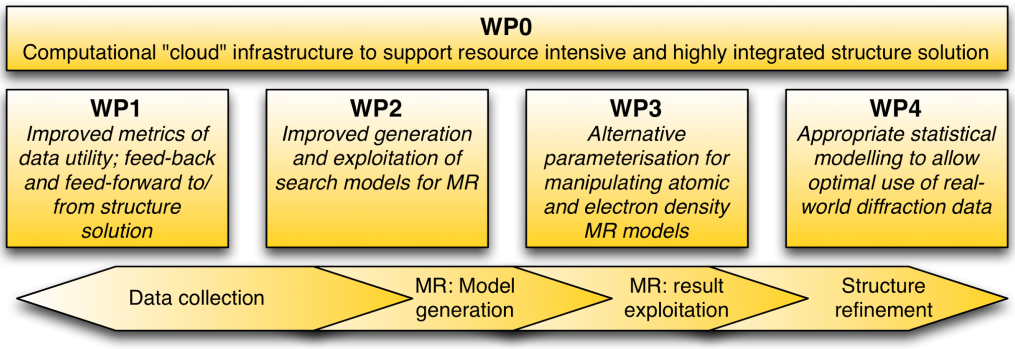
Priorities highlighted in WG1 have informed both the final scientific focus of the (successful) BBSRC/MRC grant application, and funding decisions taken by executive committee through 2013. These commitments, and the protocols by which we are trying to tighten up our decision making process around funding are on the agenda of this year's meeting.

2 Finance

The attached summaries detail how CCP4's finances are projected to develop over the next few years, and are based on the assumption of maintaining a constant head count (i.e. continuing employment or one-in, one-out). Our success in securing Research Council funding and the maintenance of our license income together mean that we enter 2014 in the position of being able to maintain and extend our activities.

2.1 Topic

We are pleased to announce that the BBSRC and MRC agreed to fund our application in full. We attach the scientific case in which the work packages are described. In short, we have secured support for five work packages, inter-related as illustrated below:



3 Scientific progress

3.1 CCP4 6.4.0

Exploiting the streamlined build, test, and distribution systems described last year, the core team have brought out version 6.4.0 of the suite. Notable additions include a centrally supported and up-to-date version of Coot, and provision for near-term inclusion of centrally-distributed versions of CCP4MG and GUI2.

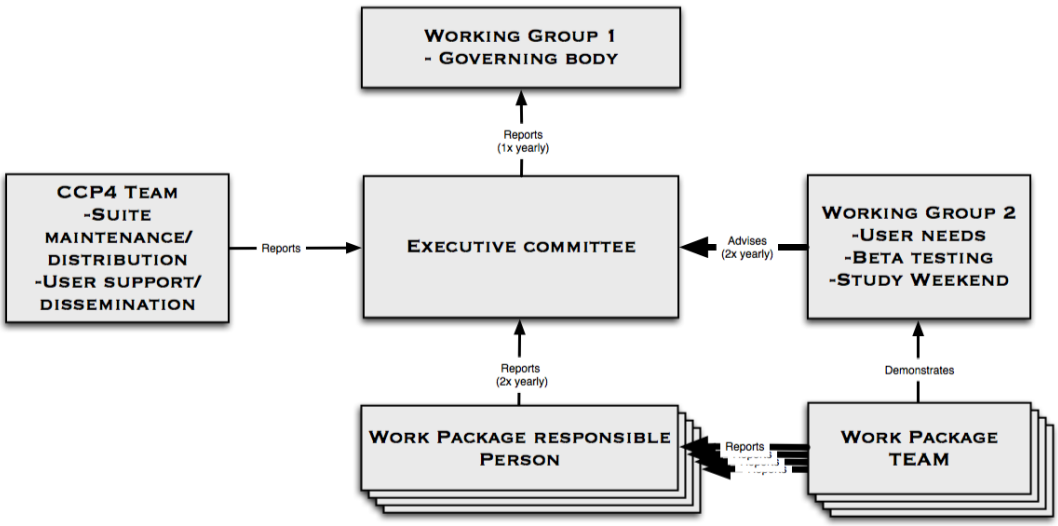
3.2 User interface

Following alpha tests through Working Group 2 and at Newcastle University, we are pleased to announce that a Google-style "by invitation" steady roll out of GUI2 will take place through January. The suite's principal architect (Liz Potterton) and the out-going chairperson (Martin Noble) will be demonstrating the suite in the lunch time bytes and in the final session respectively. The extended timeline of the roll out has allowed us to introduce some compelling features for both users and developers: we think you're going to like it.

4 Other business

4.1 Management

As ever, we are constantly looking at how to improve the effectiveness of management of the suite. The incoming chair will be working at improving the formal reporting structures of the collaboration, and we have used the new grant to review this aspect of our operation. The following illustrates the structure that we plan to use for integrating scientific management of the new grant with the committee structure of CCP4. In addition, for this and future grant applications we have set the precedent of including PI time in the grant costs, hopefully ensuring that host institutions will understand the significance of the contributions of the scientists who contribute to the suite's growth.



Executive committee Composition Chairman: M Noble, (Newcastle -2014), D Brown, (Kent, 2014-)	WP Responsibles
Ex officio: Manager: K Wilson (York) WG2 Chair: P Evans (MRC-LMB, -2014, A Pearson (Leeds, 2014-) CCP4 Core group Leader: E Krissinel (RCaH) PSDI Nominee (industry) Diamond nominee: G Evans (DLS) Elected/Co-opted members: E Dodson (York) G Murshudov (MRC-LMB) K Cowtan (York) M Winn (STFC) R Read (CIMR)	WP0: E Krissinel (RCaH) WP1: D Stuart (DLS), G Evans (DLS) WP2: R Read (CIMR), D Rigden (Liverpool) WP3: K Cowtan (York) WP4: G Murshudov (MRC-LMB)

4.2 Thanks

It has been a privilege and a pleasure to hold the office of Chairperson of CCP4, and I would like to note my thanks to Keith Wilson (CCP4 manager), the Executive Committee, the CCP4 development community, and the administrative team and core team members of CCP4 for making the time spent feel both useful and (almost invariably) enjoyable.