WG1, January 4th 2013: Minutes

Present: Apologies. No attendance list was recorded this year.

The agenda followed the items of the Chairman's report

0. The minutes of the January 2012 meeting were accepted.

1. Progress in respect of resolutions from the last WG1 meeting
The items as presented in the Chair's report were briefly discussed. No actions arose.

2. Finance
Charles Ballard's finance summary was presented by KSW. We currently have a substantial underspend and carryover due to late filling of several posts. This can help us in case of reduced level funding in the grant renewal. Once we know the outcome of the grant, then it should be possible to fund 1 or 2 time limited contracts on agreed topics.

3. Grant renewal
Plan of action from Chair's report. We will go for the April deadline. MN and new Chair when elected to be applicants to ensure continuity. Proposal preparations to start straightaway. Final discussions to take place at the Cosener's meeting in March.

4. Scientific Progress
As covered in Chair's report. Fantastic progress with update mechanism.
Congratulations to Eugene and team.

5. Other business
As covered in Chair's report.
WG2 Chair will be subject to nominations – please send to Keith Wilson. Arwen Pearson elected as Chair subsequent to meeting.

6. Study weekend 2012 and 2013.
As stated in Chair's report. The 2012 study weekend was organised by Johan Turkenburg and Katherine McAuley and was an extremely stimulating meeting where we were offered some exciting visions for the future of crystallography. 2012 also saw a passing of the baton in the organisation of the South-of-Britain BCA/CCP4 Summer School from Elspeth Garman to Airlie McCoy. With excellent support from staff at DLS (an especial thank you to Alun Ashton), the meeting proved another scientific and social mega-success.
This year's Study Weekend is organised by Helen Walden and Pietro Roversi, and will cover the ever-young topic of Molecular Replacements. It is customary for us to note our appreciation of the organisers of these meetings.
WG2 will identify the topic for 2014.

7. Election of a chairperson to take up office in 2014
The major item of the meeting. Previous plan.

- *MN to serve until January 2014, so as to see the new grant proposal through. MN emphasised he would not stay on beyond 2014.*
- *At the January 2013 WG1 should elect a new Chair to track MN during 2013, as MN tracked the last change of Chair. Nominations would be sort in the third quarter of 2012.*

- *It was agreed that the Chair tenure should in general be for 1 years tracking, to be followed by 5 years in post to see through the 5-year grant cycle.*

This is an election for the successor of the current chairperson, who will shadow the current chair through 2013 and take over as soon as the granting process permits. In a break with previous practise, we plan to make the new appointee a joint PI on the renewal grant application. There were no nominations prior to the meeting. KSW was tasked with organising nominations and a vote by mid January.
Subsequent to the meeting Dave Brown was nominated (by several members) and unanimously elected as Chair for 2014-2019.

8. Discussion: portfolio of priority projects within CCP4

There was a wide-ranging but brief discussion based on the topics in Appendix 1.
The focus of the grant was confirmed as a collaborative proposal with Diamond to cover optimum use of data.

9. Omitted item: composition of Executive Committee

There was need to elect new members but time prevented this item being discussed.

Executive Committee as of January 2012

		Start	End
Martin Noble	**Chair CCP4. Elected.**	**Jan 2010**	**Jan 2013**
Peter Moody	**Elected. Ex officio for 1 year overlap for 2012.**	**Jan 2009.**	**Jan 2012**
Frank von Delft	**Elected. Jan 2010**	**Jan 2010**	**Jan 2013**
Arwen Pearson	**Elected**	**Jan 2012**	**Jan 2015**
Dave Brown	**Industrial representative**	**Jan 2012**	**Jan 2015**
Gwyndaf Evans	**C-opted. DLS representative**	**Jan 2012**	**Jan 2015**
Phil Evans	**Ex officio. Chair WG2**		
Keith Wilson	**Ex officio. Scientific Coordinator CCP4**		
Eleanor Dodson	**Co-opted**		
Garib Murshudov	**Co-opted Jan 2007. Previous Member.**		
Kevin Cowtan	**Co-opted**		
Randy Read	**Co-opted**		
Martyn Winn	**Co-opted: STFC representative**		

Executive committee subsequently decided that FvD should continue as an elected member during 2013, with an election at the 2014 WG1 meeting.

Chair's report to WG1, January 4th 2013.

1 Progress in respect of resolutions from the last WG1 meeting

1.1 Discussion and vote: That CCP4 and Diamond work together for a coordinated theme to the renewal application

We have worked closely with Diamond to prepare an application for the grant renewal that addresses current and anticipated challenges in macromolecular crystallography, and that seeks to realise maximum advantage from our co-location with the Diamond Light Source (see below).

1.2 Discussion and vote: That the Executive Committee should contain a nominated representative from the Diamond Synchrotron

We welcome Gwyndaf Evans as a co-opted member of the CCP4 executive committee.

1.3 Discussion and vote: On election of a WG1 member to the executive committee

We welcome Arwen Pearson as a new member of the executive committee, drawn from WG1.

1.4 Discussion and vote: Guidelines for eligibility and extent of CCP4 meeting support

We have applied the guidelines to funding requests through 2012.

1.5 Discussion: portfolio of priority projects within CCP4

We have used the guidance received from WG1 in three ways. Firstly, we have included important themes suggested by WG1 in the new grant application. Secondly, we have funded a postdoctoral position to work with Garib Murshudov, Paul Emsley, and Eugene Krissinel on the handling of small molecules. Thirdly, we have drafted the attached list of possible priority areas to be discussed at this meeting, and to guide our subsequent use of CCP4 commercial income

2 Finance

The attached summaries detail how CCP4's finances are projected to develop over the next few years, and are based on the assumptions of 1) Maintaining a constant head count (i.e. continuing employment or one-in, one-out), and 2) No new income (i.e. not assuming a successful grant application)

3 Grant renewal

3.1 Topic

In line with the guidance we received from WG1, we have prepared a grant outline (attached) that seeks to coordinate CCP4 activities with software development in Diamond, especially to take advantage of synergies between the software resources of CCP4 and the experimental and computational services available at the Diamond Light Source.

3.2 Vehicle

Following on from discussions at last WG1, executive committee evaluated different vehicles for grant renewal. Colin Miles, our principal point of contact within BBSRC, indicated that their preference would be for BBSRC to act as lead agency in a joint application to BBSRC and MRC, as has been the case for recent grants. While we initially started to work towards a LoLa application for the 2013 pre-application deadline, decisions within BBSRC have changed this plan. Specifically, BBSRC will only be making LoLa grants to applicants within their specified strategic areas, into which we are told CCP4 does not fall. As such, we will instead be applying for a conventional responsive mode program grant. This has two main implications: 1) the total sum applied for must be less than the £2M limit of the LoLa scheme, and 2) the timeline for the process is substantially compressed, involving an April 2013 deadline for a full application, with a funding decision in October 2013.

4 Scientific progress

The attached summary of progress by CCP4-supported developers is a further demonstration of the strength of software development within the collaboration. Although it is invidious to single out particular accomplishments, we are particularly keen that WG1 members should be aware of the following:

4.1 Update mechanism

We have received overwhelmingly positive feedback about the autoupdate and version management tools that the core team have integrated into CCP4i. These provide a vigorous environment (10 updates in the three months since release) where users can access the latest and greatest enhancements of the suite in an automated way. **Please ensure that your staff are taking advantage of this feature…it's great.**

4.2 User interface

As we were bringing CCP4i2 to distribution readiness, we realised that we should take advantage of the roll-out to address a long standing complication of CCP4 use, namely the unnecessary mystification of computational crystallographic tasks by the (often historically dictated) file structures that are involved. We believe that we have found an exciting and intuitive solution to this challenge, with a very small activation energy barrier, which will make the conduct, automation, and teaching of crystallography substantially easier. Alpha testers will be active up to March 2013, for a staged release over the following six months. In the meantime, the core team have been anticipating aspects of this work in the form of an updated mechanism for presenting reports from CCP4i1. This too is beautiful, and offers an immediate glimpse into a more user-focussed interface that will be available from the middle of 2013.

5 Other business

5.1 PiMS

Despite the technical accomplishments of the PiMS team, take-up, especially from our commercial license holders, remained limited. While our judgement is that the project has delivered an excellent set of functionality, we are not able to resource the investment needed to complete the development and marketing of the software into a target audience composed of slow adopters. Accordingly, Chris Morris sought alternative solutions for the further development of the code. In summary, the project

has been adopted by a commercial sponsor, which will be releasing it as a standalone package. To quote extracts from Chris's explanation of the position:

"*The contract between STFC and Emerald BioSystems for the commercial distribution of PiMS has now been signed. I believe that all concerned have a real common interest in extending PiMS as new techniques are devised in academia and then taken up in industry, and in hardening PiMS so academics too benefit from commercial grade software.*
PiMS remains free for academic use, and its development for the academic community will be overseen by a board consisting of Ray Owens, myself, and two people from Emerald BioSystems.
PiMS will not be open source. No one could quite see how to make that work. Academic groups will get access to the source code, on condition that they will allow STFC to distribute changes that they make."

We hope that this arrangement is to the eventual benefit of our academic and commercial license holders, and we are grateful to Chris for his efforts in arranging it.

5.2 WG2

After providing excellent stewardship for WG2 over many…many…many years, Phil Evans has indicated that he would be happy to pass on the honour of chairing that august body to a replacement sometime in 2013. We hope to use this point in the agenda to both consider potential replacements and to listen to proposals for the future format and remit of WG2 meetings. Nominations can be sent to Keith Wilson, and will be circulated closer to the time.

6 Discussion and vote: Thanks to meeting organisers

The 2012 study weekend was organised by Johan Turkenburg and Katherine McAuley and was an extremely stimulating meeting where we were offered some exciting visions for the future of crystallography. 2012 also saw a passing of the baton in the organisation of the South-of-Britain BCA/CCP4 Summer School from Elspeth Garman to Airlie McCoy. With excellent support from staff at DLS (an especial thank you to Alun Ashton), the meeting proved another scientific and social mega-success.
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7 Election of a chairperson to take up office in 2014

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8 Discussion: portfolio of priority projects within CCP4

Please see and discuss the attached list of priority areas. Your input in this matter will be used to guide the allocation of resources over the next few calendar years.

Appendix 1 :CCP4 Strategic requirements. For discussion at WG1 2013

This document aims to stimulate a discussion of medium term priorities for support within CCP4 and by associated grants. It provides a simple statement of the overall aims of CCP4 followed by (1) a list of topics already suggested by various people to get the discussion going (2) a list of on-going activities forming part of the present portfolio of grants etc. and (3) the already agreed (by WG1 last year and Exec this year) of plans for the grant renewal.

Overall aims of CCP4

- Develop, maintain and distribute state of the art software.
- Training of users including communication of both major and minor software developments
- Promoting the next generation of developers
- Representing crystallography in wider structural biology forums
- Ensure strategy and requirements are clearly communicated to developers and wider ccp4 community

1. Suggestions of Priority areas to be discussed at WG1

These come from various people. More suggestions please, in advance if possible.

Data processing

- review all new integration packages
- XFEL data analysis
- Multi-crystal data processing

Data evaluation and QA

Low resolution structure analysis, refinement and model building

- Using data from multiple crystals for phasing and refinement/model building
- Handling low resolution data
- Refinement against unmerged data
- Atom-less models – see new grant

Ligands, and computational chemistry and cheminformatics

- Computational Chemistry and Macromolecular Crystallography.
- Use of prior information for phasing, refinement, ligand fitting and analysis (Chem- and Bioinformatics). Structural Bioinformatics and Macromolecular Crystallography: Tools to analyse macromolecular structures and recycle the knowledge accumulated in the PDB for MX analysis (including protein ligand interaction analysis)

Data from complementary techniques

- Better integration with EM (there is an MRC grant on this subject, but both parties ought to find some common ground part-way). Kevin aims eventually be able to refine EM maps against X-ray intensities. Paul is working in this area too and probably Garib.
- Hybrid methods. Simultaneous MX analysis with different experimental techniques: EM/NMR/SAX, you can add others.

Usability and workflows/pipelines beyond GUI2

- Usability - making the suite more user friendly for non-specialists, pipeliners. Workflows. This won't stop with GUI2.

Holes in our portfolio
- Substructure solution.
- Others?

Teaching.
- Is there scope for developing more teaching tools in future?
- YouTube, educational materials, tutorials

2. On-going strategic imperatives wrt grant and industrial income.

2.1 New Methods for Structure determination
- Buccaneer and …….extending lower limits of resolution required to auto-build structures.
- Model rebuilds after MR 2012
- Improved Ligand fitting 2012
- Improved refinement tools
- Low resolution refinement 2013 (already delivered?)
- Nucleic Acid building 2013

2.2 Improved data processing in MOSFLM
- Fully automated data processing
- Autoindexing multiple lattices
- Integration with pointless, aimless and truncate (QuickScale)
- Parallel processing across multiple cores

2.3 Towards an intelligent Interface
CCP4 GUI2. Significant advances demonstrated in Nov 2012. Now possible for people to visualise how this will work for users.

2.4 Suite development and Support
Software auto updates – key deliverable as discussed at Nov12 Exec.

2.5 New software for image integration: DIALS.
Collaboration with DLS and Biostruct. Project leader Gwyndaf Evans.

3. Agreed objectives for grant renewal proposal
The Strategic Areas were discuss at the last WG1 and revisited at Exec meetings in March and November 2012. Preliminary approach made to BBSRC on this basis.
WP1 Problem driven data acquisition and analysis (DIAMOND position, DI Stuart)
Data integration and analysis based on experimental requirements
WP2 Data analysis in the Cloud (Eugene Krissinel)
Cloud computing for crystallographic data analysis
WP3 Molecular models based on multiple crystal samples (Garib Murshudov)
Use of ensembles of structures from multiple experimental sources for molecular replacement
WP4 Next-generation ensembles for molecular replacement (Randy Read)
WP5 Refinement of atom-free models (Kevin Cowtan)