CCP4 WG1 minutes. 5.01.2012

Present: Martin Noble (Chair, Newcastle University), Keith Wilson (University of York), Phil Evans (LMB, Cambridge), Richard Pauptit (AstraZeneca), Mark Roe (Sussex University), Andrew Leslie (LMB, Cambridge), Gwyndaf Evans (Diamond), Dave Lawson (John Innes, Norwich), Eugene Krissinel (CCP4, RcaH), Garib Murshudov (LMB, Cambridge), Kate Brown (Imperial), Arwen Pearson (University Leeds), Simon Phillips (RcaH), Vilmos Fulop (University Warwick), Ralf Flaig (Diamond), Katherine McAuley (Diamond), Dave Hall (Diamond), Alun Ashton (Diamond), Dave Stuart (University Oxford/Diamond), Elspeth Garman (University Oxford), Dave Brown (Cangenix/University Kent), Ben Bax (GSK), Nick Keep (Birkbeck), Roberto Steiner (Kings College London), Frank von Delft (University Oxford), Helen Walden (LRI at Cancer Res UK), Paul Emsley (LMB Oxford), John Helliwell (University Manchester), Eleanor Dodson (University York), Charles Ballard (CCP4, RcaH).

1. Recruitment and Nightly build project

MN said the team was up to full strength after recent recruitments. The finance summary had been circulated prior to the meeting.

Eugene had initiated a major effort towards a better release cycle, with the first nightly builds recently made available.

2. Grant renewal

- MN suggested scientific focus on new image processing software. Multi crystals, weak images etc.
- Considerable support for this.
- Ranking of crystals (AP)
- Collaboration with Diamond essential (DIS and many others). Many MX beam lines. Software effort already within DLS.
- Pims and tracking of data from crystal to grave. MN: propose multi-funding body proposal. Set up working party to meet asap, by end of January to pursue the various bodies:

Proposal: That CCP4 and Diamond work together for a coordinated theme to the renewal application

- This was approved by WG1.
- Martin Noble/Dave Brown/Dave Stuart (WT and MRC)/Frank von Delft (SGC)/Arwen Pearson/Simon Phillips (BBSRC).

3. Executive Committee.

This was Executive as of 2010. We failed to elect new reps at the January 2011 meeting.

Martin Noble	**Chair CCP4, elected**
David Rice	**Elected. Jan 2008. Leaves end of 2010.**
Peter Moody	**Elected. Jan 2009**
Frank von Delft	**Elected. Jan 2010**
Phil Evans	**Ex officio: elected 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**

Elections at the meeting

1. The Chair thanked Peter Moody for his active contribution and asked him to remain a member for a fourth year during 2012.

2. Arwen Pearson had been nominated as an elected member by EJD, seconded by SP. Unanimous support.
3. The Chair proposed that Exec should have a co-opted DLS representative. Unanimous approval. DLS (DIS) to nominate representative.
4. The Chair reported that Dave Brown had been acting as Industry rep on Exec as agreed at the 2011 meeting, and would continue to do so for the next years. Unanimous support.

4. CCP4 Chair.

MN left the room. KSW reported that MN had been elected for a 3 years term which would formally end at the 2013 Study Weekend. KSW proposed:

- That MN be asked to serve until January 2014, so as to see the new grant proposal through.
- That at the January 2013 WG1 should elect a new Chair to track MN during 2013, as MN tracked at the last change of Chair. Nominations would be sort in the third quarter of 2012.

This was approved by WG1. MN returned and accepted this proposal – but emphasised he would not stay on beyond 2014.

A general discussion followed at which 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.

5. 2013 SW: Thanks to organisers, and topic and venue for next meeting

The Chair thanked this years organisers. The next topic was briefly discussed. Molecular replacement was suggested by PRE as the most timely topic. The organisation of the SW remains the main (sole) role of WG2.

6. CCP4 Guidelines for eligibility and extent of CCP4 meeting support

The Chair's proposed guidelines were discussed and received general approval.

7. Portfolio of priority projects within CCP4

The Chair sought ideas from WG1 for areas which might be missing from our current portfolio.

One outcome was a clear statement by Paul Emsley that the COOT Ligand handling version would be released by end of January 2012.

Richard Pauptit noted need to support for fragment work. In principle, covered by gui2 and ligands, but for the new grant proposal, the point would be the scientific case.

8. Current projects.

Amongst others the Chair focussed on the GUI2 and CCP4mg projects. He demonstrated GUI2, reported on progress, and stated we had 24 months work to do in the last 18 months of the current grant. Given the hiatus in hiring this was largely to be expected.

A new release of CCP4mg, 2.5.1, had been made just before Xmas. Much enhanced performance and stability. WG1 members were encouraged to make use of this in their laboratories.

CCP4 WG1 Meeting Jan. 5th 2012

Chairman's report

2011 Has been an important year in the evolution of CCP4, marked happily by the award of a major prize from the Royal Society for Chemistry to the collaboration as a whole. In 2012 and beyond we can look forward to reaping the benefits of important decisions that were taken over recent years in respect of 1) reorganisation of our software infrastructure, 2) recruitment to key positions in the organisation, and 3) relocation to the Research Complex at Harwell.

A root and branch reorganisation of our mechanisms for software curation, distribution, and support has been needed for two main reasons. Firstly, to shorten the delay between our developers making an important enhancement to their software (or correcting a substantial bug), and our users seeing the benefit of those developments, and secondly to provide a mechanism by which our developers might derive further benefit from working with CCP4, in the shape of automatic compilation, distribution and testing on multiple platforms. The monolithic, and often long-delayed release cycle sustained us for many years, and essential elements of it will remain as we go forward (not least to save pipeline-developers from working on an ever shifting landscape). However, all too often the requirement of assembling and testing all of the elements of our multi-contributor suite prior to release has meant that the dissemination of new features has been delayed, or that up-to-date software has not been accessible through a single and unified portal. This situation was as unsatisfactory for our developers as it was for our users.

Accordingly, Executive Committee asked WG1 to allow us to prioritise the restructuring of our software repositories and build-frameworks, with a view to allowing automatic building and testing. This year the Core Team has reached a point where a (currently platform-limited) nightly-build of the suite is accessible to the brave and/or foolish. Following a beta release of this nightly-build system in late November, we plan to publicise this mechanism to the community-at-large as a feature of the next release. Our colleagues in the Phenix consortium have benefited from a clean slate in this regard, and it is exciting to be back to a position where we too can focus on the development of cutting edge algorithms and user interaction. Another extremely positive outcome is that we are close to completing the transitioning of our Windows build onto a shared codebase and compilation system, and therefore to offering a best of breed user experience to the significant fraction of our users who are most familiar with that operating system.

Recruitment of Eugene Krissinel to the Group Leader's position at Harwell has contributed significantly to an improvement in our software management practices, and to our subsequent recruitment of technically gifted individuals with strong mathematical and computer sciences backgrounds to further enhance our Core Team. For illustration, we this year recruited:

- Ville Uski , who has a background in computational physics, and who lead the process of rationalising our software repositories and compilation mechanisms.
- Marcin Wojdyr, who has a background in computational aspects of powder diffraction, and who has lead the way with making Windows an equal partner as far as support for CCP4 software is concerned.
- Andrey Lebedev, who previously worked with Garib Murshudov in York. As well as providing the team with the insight that comes from a world-class theoretical and practical macromolecular crystallographer, Andrey is able to bridge the equally important communities of internal and extramural CCP4 developers.

Complementing the strengths of our established Core Team members, these recruits put us in a strong position to tackle meaty new challenges in computational crystallography. As such, the liberation

of our programmers from more mundane aspects of software curation, a further benefit of the software reorganisation detailed above, could not be more timely.

The relocation of our Core Team to the Research Complex at Harwell was enthusiastically supported by the majority of WG1 members, and has been completed with the help and support of STFC, Diamond Ltd, and the management and staff of the Research Complex at Harwell. While we are back to a full complement at the RCaH, hiatuses and false starts of recruitment at the new site did cost us a significant amount of momentum. Nevertheless, the decision is vindicated by the scientific possibilities that are opening up for us on this site. This year saw the release of the jointly CCP4 and Diamond-developed DIMPLE pipeline on some Diamond beamlines. This pipeline streamlines the analysis of the significant fraction of datasets that are collected for what could be called difference-Fourier purposes, i.e. to look at the local effects of a point mutation, or at the structure of a bound ligand. We have also initiated work on the next generation data analysis software that was sanctioned as a scientific priority by WG1 at the last Study Weekend. Additional FTEs for this project come from Diamond and from a Biostruct-X project at the EU, and CCP4 (through Andrew Leslie and Eugene Krissinel) and Diamond (through Gwyndaf Evans) are providing a scientific lead. We would like to extend this cooperation with Diamond, so as to maximise the benefits of our co-location, and Eugene will be working with Gwyndaf Evans and Alun Ashton to realise this ambition.

In particular, and with the consent of WG1, we would like to propose that the core theme of our application this year to renew CCP4's research council funding is centred around a coordinated development by CCP4 and Diamond. This development is to target the optimal collection, analysis, and exploitation of multiple fragmentary datasets that may contribute to the solution of a single protein structure. Scenarios where such a development is needed will be well known to WG1 members: small crystals from which damage-limited single-crystal datasets are largely incomplete; clustered and/or intergrown crystals from which processable data can be collected over only a limited rotation range; crystals with low symmetry and/or high radiation sensitivity, especially where these properties are accompanied by poor crystal-to-crystal isomorphism; cases where very many derivatives with limited dispersive or anomalous signals and/or poor isomorphism contribute to the determination of phases. Such cases present challenges that apply to:

- the hardware and software that control data collection,
- data analysis software that must quickly calculate strategies for context-aware dose-limited data collection,
- data reduction software that must handle highly incomplete data collected from multiple crystals with varying isomorphism,
- data and project management software that must curate and keep book on the partial datasets from this analysis, and
- the phasing and refinement algorithms that have to make structural lemonade from the lemon-like datasets that the process generates.

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

CCP4 is extremely serious about working together with Diamond, and we intend that this collaboration should be visible to users coming to Diamond beamlines. We are investigating mechanisms to allow Diamond visitors to take advantage of CCP4 expertise located in the adjacent building to address their software installation and crystallographic problems. We see this as being of mutual benefit to our users and our developers, since the gathering of user feedback (probably best realised at the moment in the bulletin board and in such CCP4 projects as Coot) is an essential element of identifying scientific needs, and of defining how those needs should best be met.

We also wish to ensure that CCP4 and Diamond are cooperating effectively to meet user needs by introducing Diamond representation on the CCP4 Executive Committee. We therefore propose, with WG1s consent, to allow Diamond to nominate an *ex officio* representative to the Executive Committee.

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

2011 saw the end of David Rice's fixed term on executive committee, and by the same process we should thank Peter Moody for his contribution at this year's study weekend. We used the slot liberated by David to define a new ex-officio role on exec, namely commercial license holders' nominee, a role currently fulfilled by Dave Brown.

Democratic propriety, and the excellent reasons that underlie it, demands that we should make it possible for WG1 to elect Peter's successor, and I would hereby like to solicit nominations.

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

Last year's study weekend was held in Warwick and was both well attended and well received. Once again, we would like to thank the organisers, Kevin Cowtan, Paul Emsley and Keith Wilson. The review paper on CCP4 is already generating substantial citations, 149 by late December. This year's study weekend is on the topic of Data Collection and Processing, and is jointly organised by Katherine McAuley and Johan Turkenburg, with the now usual stellar array of speakers. I would like to minute WG1s appreciation of the efforts that the meeting organisers undertake, and the role that WG2 plays in helping to define the topic and speaker list. I am sure that WG2 would appreciate any suggestions that might arise for a topic for next year's meeting.

Discussion and vote: Thanks to organisers, and topic and venue for next meeting

Possibly because of the hard economic times that prevail or, more optimistically, because of an upturn in the activity of our community, we are seeing a significant number of requests for CCP4 meeting support. While these are useful to CCP4 and to those who attend the meetings, it is now necessary to generate a set of guidelines that we can apply to consider all such approaches equally.

The attached were drafted and tweaked by exec, and we would like to have them ratified by WG1.

1) CCP4 support shall be capped at £15K, being the sum with which we are currently able to carry most of the costs of our flagship summer schools, which we jointly run with BCA.

2) Other than meetings initiated by CCP4, support will be capped at £2K, with exceptional cases being agreed by the executive committee up to a limit of £5K

3) Support will be capped at 50% of the total cost of the meeting (contributions in kind from other sources and registration fees can be factored into this calculation)

4) The support should be justified in terms of supporting the attendance of CCP4-contributing developers. Further support may be made available to enable the attendance of graduate students. The CCP4 Study Weekend and the Annual Summer School are exempt from this requirement.

5) Support shall be limited to meetings that centre on methods development or that teach current methods to students.

6) Preference will be given to meetings that are accessible to the whole community.

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

It is normal practise for us to debate and approve one of our major meeting-sponsorships, namely for the running of the annual CCP4/BCA Summer School on Computational Crystallography. Over recent years, the South of Britain Summer School was run by Elspeth Garman, with some credit also taken by Martin Noble. Last year, WG1 approved our suggestion that Airlie McCoy be invited to organise future South of Britain Summer Schools, and she has kindly agreed to do this, with help and support from Colleagues at Diamond. Despite difficult times, this has allowed her to keep projected costs low, and she has asked us for only £10K. I would like to invite a vote on the release of these funds, as well as a vote of thanks to the organizers of this years North of Britain meeting (Garry Taylor & Jim Naismith), and of special thanks to Elspeth for her contribution over many summer schools. Lest you all worry unduly, Elspeth has agreed to continue teaching on the course.

Discussion and vote: Thanks to organiser past and present, and release of funds for Summer School 2012

Project reports

We have appended below the summary achievements and targets of our fully-supported developers, and are happy to discuss the status and or future of these projects. Our main focus for the moment continues to be on the front and back-end of a pipelining and GUI framework for future user interaction with CCP4 software. Time-permitting, I would like to demonstrate a snapshot of some aspects of this work at the WG1 meeting.

Discussion: portfolio of priority projects within CCP4

Individual developer reports 2011

NAME:Charles Ballard

JOB TITLE:Scientific Programmer

2011 TARGETS: 5-10 bullets each cell

- Release 6.3.0.
- Standalone libraries.
- Development the autobuild/autotest system.
- General improvements to ctruncate.
- Recruitment of new staff.
- Workshop in Okinawa.
- Continued monitoring of the group finances. To shift more of the finance tracking, procurement, etc onto Karen McIntyre.

2011 ACHIEVEMENTS:

- Increased stability of ctruncate, along with better statistics.
- Recruitment and integration of new staff. VU has got the autobuilds working for the next release.
- Release of standalone libraries (preformed by MW).
- Pre-releases of CCP4 6.3.0.
- SSC haven't mucked CCP4 up too much.
- Workshop in Okinawa.

2012 TARGETS:

- Continued development of ctruncate to better cover data quality statistics (some parts in collaboration with AL)
- Integration of ctruncate elements into viewhkl (collaboration with EK)
- Integration of ctruncate elements into aimless (collaboration with PRE)
- Going live of developer repositories.
- Going live of autobuild/autotest system
- Release 6.3.0 (team target)
- Possible workshops in Japan and India.

NAME: Kevin Cowtan

JOB TITLE: PDRA

2011 TARGETS: 5-10 bullets each cell

- Nucleic acid building
- Buccaneer completeness scores
- CCP4i2 pipelines
- ProteinDB chain database

2011 ACHIEVEMENTS:

- Nucleic acid building
- Buccaneer completeness scores
- CCP4i2 pipelines
- Report framework for CCP4i2
- Composite omit code (not yet released)

2012 TARGETS:

- Nucleic acid sequencing
- Nucleic acid build/refine pipeline
- Release composite omit code and pipeline
- MR model improvement?
- Carbohydrates and ligands?

NAME: Paul Emsley

JOB TITLE: CCP4 Fellow: Project title: COOT

2011 TARGETS: 5-10 bullets each cell

2011 ACHIEVEMENTS:

Release 0.6.2 : 8 new features, 14 changes and 30 non-trivial bug fixes.

- Most notable change: Move to PDB v3 atom naming, new refmac dictionary.
- http://coot.googlecode.com/svn/trunk/RELEASE-NOTES
- http://coot.googlecode.com/svn/trunk/rel-todo

Release 0.7

- Bond orders used when drawing het-groups.
- 2D Ligand builder is also built into Coot now - communication is via build-in variables rather than files. Prodrg interface has been improved. Now uses prodrg+refmac for 2d ligand layout. Ligand environment analysis and hydrogen-bond representation.
- Add hydrogen-sprouting and hydrogenation of region.
- Drag and drop has been introduced into the main graphics window and the 2D canvas.
- Integration of Kevin's SLOOP/db-loop code.
- Multi-residue torsion - allowing the manipulation of the position of a residue by changing the torsions of a neighbour (e.g. moving a NAG by rotation of the chi-1 angle of the ASN).
- mmCIF parser extended to read torsion and chiral information from structures rather than loops.
- New coordinates are tested for nomenclature errors on reading.
- PDBe recent strcture browser - download coordinates, sfs cif, convert to mtz and run refmac at the press of a button. All done in subthreads so the main application is not blocked. Rework the data-handling interface to work with new clipper libs.
- Improved interface with the EDS - now we download the web page for the respective entry so that we know if the map is reliable or not.
- Solid-modelling of generic display objects and environment distances.
- Added a "What's this?" menu item to identify ligands by name (rather than simply 3-letter code). Similarly the "Add Solvent Molecule" dialog has been expanded.
- Dotted surface representation improved.
- Small-molecule cif-reader added (with the help of Eugene Krissinel).
- Symmetry-handling of transformed map improved.
- Improved navigation via keyboarding of go-to-residue.
- Added single-model view (for NMR models, for example).
- Added the ability to make LINKs.
- From now on, all binaries that I build will have python embedded.
- Implemented Hole algorithm of Oliver Smart and co-workers.
- Implemented lsq-improve algorithm of Kleywegt and Jones.

2012 TARGETS:

- Use LINKR information from refmac to identify links between residue for sphere refine and mult-residue torsion and identification of glycans.
- More improvements to the Carbohydrate/Oligosaccharide Linking tool.
- More improvements to ligand environment analysis - for example, include charge-charge interactions.
- Move to new-style SRS-usage (instead of SBase) - modern ligand database. Improved search tools.
- Improve the topological equivalence filtering (for use with PRODRG ouptput).
- Interactions with the CREDO ligand-protein interaction database for drug discovery.
- Improve ligand fitting - try multi-threaded and sampling of small translations to see if that can escape from occasional local minima.
- Use of (fixed) residues in the environment to provide "bump" restraints (so that residues/ligands don't stray into the density of neighbouring residues when those residues are not part of the refinement) useful at lower resolution, I imagine.
- Improved integration/interface with PDBe services and validation information (VTF-info).

NAME: Owen Johnson

PROJECT TITLE: iMosflm maintenance and development

2011 ACTIVITIES:

- Improved interface speed and memory overhead when integrating many images.
- Improved Strategy pane for calculations from multiple segments & crystals; now includes space group selection.
- Improved response of the Image display pane by minimizing requests to Mosflm for calculation of predictions for redisplay; implemented FindHKL function as top-level widget with 'success' icon; added display of bad spots on images.
- Added re-checking & optional re-setting of initial detector and crystal parameters should they refine to unreasonable values; added advanced integration options to treat outliers affected by ice rings in Mosflm.
- Continued interface bug-fixing & strengthening throughout; overhauled tutorial document & images therein.

2012 PLANS: (to end of current grant: 18 April 2012)

- Continue work to improve speed of integration for many images.
- Continue bug-fixing & general strengthening of the interface.

NAME: Ronan Keegan

JOB TITLE: Computational Scientist CCP4 Group

2011 TARGETS: 5-10 bullets each cell

- Successful release of CCP4 6.2.0
- Incorporation of AMPLE software into CCP4 repository system for future release including the develop CCP4i interface
- Incorporation of DIMPLE software into the CCP4 repository system
- Recruitment of core CCP4 staff and management of one new member with responsibility for Windows
- Tender and purchase of CCP4 compute cluster facility
- Organisation of 4th annual CCP4/APS Summer School in protein crystallography

2011 ACHIEVEMENTS:

- CCP4 6.2.0 release
- Development of AMPLE software and first novel structure solved using this software
- Organisation of successful CCP4 Schools at the APS in Chicago, Harvard Medical School and Okinawa, Japan
- Oversee the organisation of the CCP4 SW at Warwick University
- OpenMP parallelisation of the Aimless program
- Purchase and commissioning of CCP4 cluster hardware for CCP4 webservice facility at RCaH
- Continued development and maintenance of MrBUMP software
- Update of Windows build mechanism for CCP4 and overseeing of CCP4 core staff effort on this project

2012 TARGETS:

- CCP4 6.3.0 release
- Development and release of AMPLE software in CCP4 Suite in collaboration with University of Liverpo
- Development and release of DIMPLE software in CCP4 Suite in collaboration with Diamond computatio
- Development of update mechanism for CCP4 suite
- Continued development of MrBUMP software
- Management of core CCP4 staff
- Organisation and running various CCP4 educational outreach events (APS School, CCP4 SW)
- Investigate refinement of ensembles in Refmac
- Contribute to CCP4 release cycle
- Contribute to CCP4 modernisation project

- Deployment of CCP4 related webservices on CCP4 cluster

NAME: Eugene Krissinel

JOB TITLE: CCP4 Group Leader

2011 TARGETS: 5-10 bullets each cell

- day-to-day direction of group activities
- raising group to normal staff level
- representation of group at departmental level
- coordination with Diamond software groups
- development of plans for, and initiation of the CCP4 Release Cycle Modernisation Project
- participation in Helpdesk activities
- coordination with CCP4i2 and CCP4mg developers
- coordination with Coot and Refmac teams on ligand support framework
- own software developments and support
- participation in CCP4 workshop programmes and international conferences

2011 ACHIEVEMENTS:

- group activities are monitored and conducted through regular release and development meetings
- 4 staff members recruited
- coordination with Diamond software group achieved through regular meetings and progress monitoring of joint developments
- plans for CCP4 Modernisation Projects developed, the Project started immediately after the recruitment of new staff, progress monitored
- development of CCP4mg is coordinated through regular review meetings and development of working plans
- new framework for ligand data support is developed and adopted for PISA and new PDB2->PDB3 converter; the framework will be adopted by Coot as well
- new graphical MTZ browser (viewhkl) developed and scheduled for release
- new structure alignment software (Gesamt) developed and scheduled for release
- new ligand-handling features are added to PISA, released
- lectured and tutored at 2 CCP4 International Workshops/Schools
- delivered 4 invited talks at international conferences and workshops
- 2 papers published

2012 TARGETS:

- day-to-day direction of group activities
- representation of group at departmental level
- continuing coordination with Diamond software groups
- pursuing the CCP4 Release Cycle Modernisation Project
- participation in Helpdesk activities
- coordination with CCP4i2 and CCP4mg developers
- pursuing coordination with Coot and Refmac teams on ligand support framework
- own software developments: advanced viewhkl featutres and enhancement of ligand support in PISA
- participation in CCP4 workshop programmes and international conferences

NAME: Andrey A. Lebedev

JOB TITLE: Scientific Programmer

2011 TARGETS: 5-10 bullets each cell

- ccp4i2 task for Refmac.
- ccp4i2 task for Molrep (Patterson, in-density and multi-copy searches).
- Proposal for an alternative CCP4 GUI design.

- Paper on JLigand.
- Presentation at IUCr congress.
- Integration of JLigand and Zanuda into ccp4i1.
- Teaching at APS workshop.

2011 ACHIEVEMENTS:

- ccp4i2 interface for Refmac.
- ccp4i2 interfaces for Molrep (Patterson, in-density and multi-copy searches).
- Proposal for an alternative CCP4 GUI design.
- Paper on JLigand.
- Presentation at IUCr congress.
- Integration of JLigand and Zanuda into ccp4i1.
- Teaching at APS workshop.

2012 TARGETS:

- Miscellaneous tasks for ccp4i2.
- Experimenting with macromolecular crystal structure solutions using Phoenix and my collection of test cases.
- ccp4i1/ccp4i2 report pages for major ccp4 components.
- Integration of JLigand and Zanuda into ccp4i2.
- JLigand development: (i) graph-based algorithm for descriptions of modifications, (iii) automatic assignment of monomer type (peptide, nucleotide, pyranose), (iv) use of alternative regularisation program. e.g. ProDrg.
- Analysis on prospects of JLigand and restraint library development.
- Twin law determination in Refmac, Sfcheck, Ctruncate: use of obliquity for scoring operators instead of mean deviation of bond lengths.
- Presentation of Zanuda at CCP4 Study weekend.
- Documentation and report in CCP4 news letters on Zanuda.
- Teaching at APS workshop.

NAME: Karen McIntyre

JOB TITLE: CSE Administrator

2011 TARGETS: 5-10 bullets each cell

- Updating the CCP4 licencing database as required with amendments for current and new licencees.
- Raising invoices for CCP4 licence maintenance in April and September. Liaising with Joanne Basnett (CSE retained finance) regarding payments etc.
- Processing initial enquires from potential licence holders.
- Helping with travel, accommodation etc for members of group and others with regard to meetings, conferences etc.

2011 ACHIEVEMENTS:

- Chasing up commercial licence holders for payment of licence fees (sometimes going back a number of years) – now much less money outstanding. This included getting money that referred to companies that had been taken over from the new company owners i.e. Organon from Merck.
- Keeping eye on income from CCP4 licence fees across years so know what money has come in from which year, income each year etc for Charles.
- Learning a little bit of html so could edit APS school part of CCP4 webpages (under instruction from Ronan) when required.
- Helping Shirley Miller with some aspects of CCP4 study weekend. This included requesting invoices as required, checking accommodation details for certain dates, arranging receipts etc so that she could get on with the bigger things that needed to be done.

2012 TARGETS:

- Updating the CCP4 licencing database as required with amendments for current and new licencees.
- Raising invoices for CCP4 licence maintenance in April and September. Liaising with Joanne Basnett (CSE retained finance) regarding payments etc.
- Processing initial enquires from potential licence holders.
- Helping with travel, accommodation etc for members of group and others with regard to meetings, conferences etc.
- Assisting with the arranging of workshops and conferences.

NAME: Stuart McNicholas

JOB TITLE: Postdoctoral Fellow, University of York working on CCP4MG

2011 TARGETS: 5-10 bullets each cell

- Status file improvements: implement in XML, collaborate with Brian Marsden of SGC on file formats; make some program options user preferences which are not saved by default.
- Normal mode visualisation as dynamic movie and static porcupine representation.
- Rationalization of symmetry generation, and more user friendly and useful symmetry options.
- Sequence viewer improvements. More graphical views of alignment results.
- Shadows in graphics window.
- Ambient occlusion in graphics window.
- Textures in graphics window and render module.
- Define plugin API.
- Coordinate editing tool.

2011 ACHIEVEMENTS:

- Implemented normal mode visualization as animations and porcupines.
- Made major improvements in the speed of drawing objects in OpenGL, this also causes speedup when drawing symmetry as defined from CCP4MG "Crystal" objects, but not "Generate symmetry mates". Fixed serious bugs drawing lipid cartoons.
- Fixed many serious memory leaks and crashes.
- Improvements in OpenGL and render module shaders.
- Implemented vizualization of ProSMART results in CCP4MG.
- Written loggraph replacement.
- Written infrastructure so that plugins can create custom colouring schemes and drawing styles. Used by Sequence Viewer to colour by conservation, Normal Modes to colour by mobility and define porcupines and to colour by ProSMART Still needs to be documented.
- "Circles" drawing method.
- Some sequence viewer improvements: delete sequences, undo alignment, cope with some slight variants in clustal format.
- Added some saner scaling and view orientation options to picture definition file for easier interoperation with CCP4i2.
- Started collaboration with Brian Marsden of SGC on standardizing molecular graphics file format.

2012 TARGETS:

- Threading to offload expensive taks to keep GUI responsive.
- Named atom selections and concept of active selection.
- Bond order representation.
- XML status file.
- Vizualization of angles, dihedral angles, etc.
- Lipid membrane representation.
- MG as an widget embeddable in other programs.
- Coordinate file editor which can talk to i2 database.
- Electron density rendering done as vertex arrays/VBOs.

Chris Morris

ACTIVITIES Dec 2010 TO PRESENT

Take up: The Naismith group, St Andres; Noble/Endicott groups, Newcastle; University of Sao Paolo; University of Oklahoma; Charles University, Prague. There are 21 licenced installations.

Activities:

- Delivered PiMS 4.2, including support for synthetic genes.
- Developed support for Rhombix instruments.
- Working with DLS on reimplementing e-HTPX web services, especially with a view to supporting in-plate screening for MPL.
- Supported the INSTRUCT hosted PiMS service, which has now been relocated to DL.
- Tutor on Protein characterization and crystallization course, **May 2-6, 2011**, University of Helsinki, Institute of Biotechnology.

Resources:

Chris Morris is funded by CCP4, to July 2013. Jon Diprose contributes some code to PiMS/xtalPiMS. Ed Daniel is employed by the University of Oulu to install xtalPiMS and extend it.

Publications:

"The Protein Information Management System (PiMS) : a generic tool for any structural biology research laboratory" Acta Crystallogr D **67** (4) 249-260 (2011) [doi:10.1107/S0907444911007943]
E Daniel , B Lin , JM Diprose , SL Griffiths , *C Morris* , IM Berry ,et al (4)
xtalPiMS: a PiMS-based web application for the management and monitoring of crystallization trials
Journal of Structural Biology 175 (2011) 230¿235 [10.1016/j.jsb.2011.05.008] [application/pdf]
M Savitsky ,JM Diprose ,*C Morris* , SL Griffiths , E Daniel , B Lin , et al (7)
Recording information on protein complexes in an information management system
J Struc Bio **175** (2) 224-229 (2011) [10.1016/j.jsb.2011.05.009] [application/pdf]
J A Segal, *C Morris*
Developing software for a scientific community: some challenges and solutions
in Handbook of Research on Computational Science and Engineering: Theory and Practice, eds. Joanna Leng, Wes Sharrock (IGI-Global) (2011)
JA Segal, *C Morris*
Scientific end-user developers and barriers to user/customer engagement
JOEUC **23** (4) 50-62 (2011) [DOI: 10.4018/joeuc.2011100104]

PLANS TO Dec 2012

- Organise CECAM Collaborative Scientific Software Development meeting on "Integrated software for integrative structural biology" – funding is now confirmed.
- Deliver improved support for mutagenesis, as specified by Noble/Endicott groups.
- Deliver improved support for HTP work using cohorts of targets, as specified by OPPF-UK.
- The BioMedBridges includes 6 person months to STFC to contribute to standards for data exchange, and a 40 person month post to allow joint searching of PiMS and other biomedical databases.
- DLS is considering commissioning CM for 6 person months to write a new web app to give users access to data in ISPyB, and diffraction images.
- Continue gathering requirements for bioinformatics for construct design – this may be a priority in 2013.

DEPENDENCIES

Collaboration with DLS.

NAME: Liz Potterton

JOB TITLE: CCP4i2 GUI, Database, Pipeline Development

2011 TARGETS: 5-10 bullets each cell

- Work with pipeline developers to create pipelines and program wrappers to be used in GUI
- Develop data classes and widgets for more complex crystallographic data
- Develop project database (based on ZODB) and infrastructure and user interface for managing

projects and jobs.

2011 ACHIEVEMENTS:

- Some wrapper, data object and widget development, mostly with Martyn Winn and also with Andrey Lebedev.
- Developed project database based on SQL (ZODB was not sufficiently stable) and a Python API.
- Developed a GUI interface to the project and incorporated with existing interfaces to tasks. Has been much discussed by a 'GUI Forum'.
- Developed a report generator (a 'better Baulbes') based on code by Kevin Cowtan.

2012 TARGETS:

- Improve user experience of GUI based on feedback from GUI Forum and others.
- Work with other developers to create interface to all necessary crystallographic functionality.
- Release version 1 incorporated in CCP4 Suite.

NAME: Harry Powell

JOB TITLE: Mosflm

2011 TARGETS: 5-10 bullets each cell

Mosflm: Improved handling of multicircle goniostats (including automated setup from image headers). Finish coding automatic backstop location. Improve robustness of parameter refinement. Implement these features in fully automated data processing.
User support, teaching at crystallography schools, bug fixing. Start looking at re-factoring code.

2011 ACHIEVEMENTS:

User support, teaching, bug fixing etc fulfilled.
Multicircle goniostat implementation being re-engineered by David Waterman.
Automatic backstop code works okay some of the time – backstop arm location is still problematic especially with tiled detectors (give rise to false edges), but not implemented in iMosflm. Added code to smooth over several images, but still not robust.
Added fast decompression for Pilatus – runs ~20X faster than CBFlib.
Worked through MINGW cross-compiled build again, using gcc 4.4 – gcc 4.6 so that we can use F95 optimisations. Passed on info to central CCP4 devs.
Improved mosaicity estimation code.
Started looking at re-factoring code.
Organised IUCr Computing School.

2012 TARGETS:

Making multiple lattice indexing work more generally, particularly for closely aligned lattices; look at implementation of refinement & integration of multiple lattices in code.
Iron out problems in backstop location.
Make generalised code from David Waterman easily available to users.

NAME: Ville Uski

JOB TITLE: scientific programmer

2011 TARGETS: 5-10 bullets each cell

- participate CCP4 release 6.3.0 compilation and testing
- implement mock download pages for the suite, incorporating optional download of ARP/wARP (in collaborations with EMBL Hamburg)
- deploy Buildbot and Bazaar repository system
- implement a Nightly Builds web site
- test Bazaar repository system for use within CCP4 community

2011 ACHIEVEMENTS:

- bundled a new test release 6.2.991
- implemented mock pages to download ARP/wARP, with a protocol agreed with EMBL Hamburg
- made Buildbot run the autobuild scripts on Linux and Mac
- created a web page which dynamically maintains a list of nightly builds, automatically compiled using Buildbot and the autobuild scripts
- tested and wrote a report on Bazaar. Converted a part of the CCP4 source repository from CVS to Bazaar.

2012 TARGETS:

- implement new download pages, based on the mock pages and further discussions with the CCP4 team
- implement test environment for the suite, preferably using the Buildbot API
- deploy Buildbot on CCP4 cluster
- convert the whole CVS repository into a Bazaar repository, or agreed otherwise
- investigate CCPForge or similar system to be used as developer website for CCP4
- implement free R value with resolution bin, initially within the current FreeRflag program. Confirm correct handling of lattice symmetry in generation of current free R.
- contribute to CCP4 modernisation

NAME: David Waterman

JOB TITLE: Scientific Programmer

2011 TARGETS: 5-10 bullets each cell

Major project work, with supervision from Andrew Leslie (LMB-MRC Cambridge):

- Research and design of generalised goniometry and refinement routines for diffraction image integration software
- Implementation of these routines in the CCP4 program MOSFLM
- Liaison with BioStruct-X WP6 contributors regarding use of generalised routines by future integration software

Project work within the modernisation aims of the CCP4 suite:

- Development of Python dispatchers for a platform independent system to provide encapsulation of the CCP4 environment just prior to program execution

Ongoing core activities, including:

- Support for users of the suite
- Debugging of CCP4 software
- Plans and design for future releases, maintenance of CCP4 resources (web site, mailing lists etc)
- Presentation of CCP4 at conferences

2011 ACHIEVEMENTS:

- Review of definitions and mathematics for generalised spot coordinate prediction and derivatives with respect to a model parameterisation for integration software
- CCP4 representation at the BioStruct-X WP6 kickoff meeting
- Completion of working prototype dispatcher generator
- Settling into CCP4 core duties quickly, having begun work as a new starter in March
- Manning the CCP4 stand plus poster presentation at the IUCr Madrid

2012 TARGETS:

- Begin work on BioStruct-X integration software project, under instruction from the project manager. Initial activities are likely to be related to design and implementation of a framework in the form of an underlying library. Later focus will shift to development of modules to plug into this framework for specific tasks

such as novel algorithms for improved integration and error estimation.
- Complete derivation of the normal equations for new parameter refinement routine in MOSFLM and procedure to solve these in a robust way (using eigenvalue filtering)
- Implementation of parameter refinement routine in MOSFLM
- Integration of the dispatchers with the suite installer(s)

NAME: Keith S. Wilson

JOB TITLE: Scientific advisor to CCP4

2011 TARGETS: 5-10 bullets each cell

- Working with the Executive and Eugene towards the recruitment of new staff. In 2011 this will focus on completion of the recruitment cycle for the three core posts and the proposed new project on image processing software.
- Visits to RcaH to contribute to the planning of activities with the core team.
- Advising the team leader, Dr Eugene Krissenel.
- Regular contacts with CCP4 funded staff at Universities or other institutions.
- Contributing to Working Group 1 (WG1) and Working Group 2 (WG2).
- Assisting in the setting up of the recruitment of appropriate staff for the CCP4 team and for external appointments, in collaboration with the core team, the executive.
- Planning and coordinating the annual developers meeting at Cosener's in March/April, with the core team.
- Planning and coordinating meetings of the CCP4 Executive committee.
- Planning and coordinating developers meetings as required, focussed on GUI2 this year.

2011 ACHIEVEMENTS:

- Successful recruitment of three new staff, A Lebedev, M Wojdyr, V Uski to the core team.
- Recruitment of David Waterman on a one-year contract to kick-start the Biostruct project on a new data collection suite in collaboration with Diamond.
- Start-up of the Biostruct project discussions with Gwyndaf Evans. The EC part of this project is now funded to start in 2011.
- Establishment of new contracts for Liz Potterton and Stuart McNicholas for 3 years, Stuart to work primarily on ccp4mg, but making contributions to the GUI2 project through loggraph etc. Liz to continue her work on GUI2.
- Organisation, with Eugene, of the Cosener's meeting in April.
- Organisation of the GUI2 forum meetings in the second half of 2011.

2012 TARGETS:

- Organise the Cosener's meeting.
- Organise regular meetings of the GUI2 forum.
- Work with Eugene to plan how we can best exploit all the new talents in the core team to really advance CCP4 and not just carry out routine support work.
- Work with Stuart to advance the capabilities of CCP4mg.
- Develop a more effective way of having regular exec input to CCP4's activities.
- Advising the team leader, Dr Eugene Krissenel.

NAME: Marcin Wojdyr

JOB TITLE: scientific programmer

2011 TARGETS:

n/a

2011 ACHIEVEMENTS:

- new installer for Windows (for now available at ftp://ftp.ccp4.ac.uk/mww/)
- updated build of Tcl/Tk w/ libraries (users do not need to download ActiveTcl anymore)
- the suite can be compiled with MinGW (GCC on Windows) compiler (at least there are no known problems),

- (in progress) explored different building systems (cmake, automake, scons) and possible ways of packaging, distributing and updating of the suite. This was partly side-effect of the previous point. Scons, used by cctbx, needed to be enhanced. The same with automake-based scripts. I used cmake to build Fortran code (it's simpler than automake and scons and more flexible then set of makefiles).
- fixed a few spotted bugs

2012 TARGETS:

- learning about protein crystallography to know what our suite is for
- coding: enhancing DIMPLE (difference map pipeline)
- contribute to CCP4 6.3.0 release (Windows)
- (in progress) alternative way of distributing software for Linux: distro-specific packages. First, Coot with dependencies (mmdb, libccp4, clipper) will be packages for ~20 popular distributions using Open Build Service. If successful, it can be extended to the whole suite.

Appendix
Letter of request from Airlie McCoy