

The WG1 Meeting was held at 9.00 - 10.45 on Sunday 4 January 2009 in Conference Suite 4 a/b in the Nottingham Conference Centre

Present

Present.

Jim Naismith (St. Andrews – Chair)
Keith Wilson (York - Secretary)
Lindsay Sawyer (Edinburgh)
Garry Taylor (St Andrews)
Phil Evans (MRC-LMB)
John Helliwell (Manchester)
Leo Brady (Bristol)
Elspeth Garman (Oxford)
Frank von Delft (Oxford)
Neil Isaacs (Glasgow)
Andrea Hadfield (Bristol)
Vilmos Fulop (Warwick)
Peter Moody (Leicester)
Kate Brown (Imperial)
Nicholas Keep (Birkbeck)
Richard Pauptit (AstraZeneca)

Kevin Cowtan (York)
Adrian Laphorn (Glasgow)
Tadeusz Skarzynski (GSK)
Mark Roe (ICR)
Eleanor Dodson (York)
David Stuart (Oxford)
Andrew Leslie (MRC-LMB)
Jenny Littlechild (Exeter)
Arwen Pearson (Leeds)
Tom Edwards (Leeds)
Thomas Sorensen (DLS)
Ralf Flaig (DLS)
Charles Ballard (STFC)
Martyn Winn (STFC)
Chris Morris (STFC)

Apologies David Rice, Simon Phillips

1 Minutes of previous meeting were accepted. These had been circulated the previous January and were available on the web (<http://www.ccp4.ac.uk/wg>).

2 Matters arising: None not covered elsewhere.

3 Chairs report (Appendix 1)

The meeting recorded thanks to Randy Read and Gerard Kleywegt for organising such a successful meeting last year.

The meeting recorded thanks to Clemens Vornrhein (Global Phasing), Arwen Pearson (Leeds) and Elspeth Garman (Oxford) for undertaking to organise this meeting. Thanks also to Shirley Miller Damian, Tracey and Laura for their help with the organisation. XXX Surnames please

WG1 noted its thanks to the core staff Martyn Winn, Charles Ballard, Ronan Keenan, Norman Stein, Graeme Winter, Peter Briggs & Francois Remarclé. WG1 wished Graeme, Peter & Francois well in their new positions.

WG1 was pleased to note the release of V6.1, although expressed its desire to make sure the suite keeps pace with developments in component programs.

WG1 was pleased the grant was renewed. It made clear its desire to continue to seek research council support. WG1 thanked all those who contributed to the grant.

WG1 agreed a rise of 500 GBP for a full licence from Jan 2010 (approx 5%), with a pro-rata increase for the subsidiary license

WG1 discussed the state of the suite at length. While pleased with the progress, it was keen to see further improvements across the board. PHENIX has proven a spur to development. WG1 agreed that support for Irix could be dropped and suggested that only the main flavours of linux were supported. WG1 requested that a mock up of the new GUI be presented by Liz Potterton at the next WG1 meeting, and that she undertake visits to academic and commercial organisations to gather requirements and feedback. Several institutions expressed interest in hosting these sessions.

WG1 expressed its desire to see outreach targeted to students and new entrants into MX within the UK. There was no great desire to become a sponsoring organisation. Those involved in organising such activities are greatly appreciated by the whole community.

WG1 expressed its support for the move to RAL but noted its concern over the effects on the suite.

Kevin Cowtan left the room at this point.

There was a wide ranging discussion of Kevin Cowtan's position with respect to future CCP4 funding. The following points were agreed

- (1) Kevin Cowtan has been and is an outstanding scientific programmer
- (2) CCP4 in particular has benefitted enormously from his selfless commitment to share the fruits of his work
- (3) His intellectual contribution to the grant was recognised, the new programs he is developing are world leading.
- (4) WG1 unanimously approved the executive proposal that CCP4 make a deferred offer of a five year CCP4 fellowship to Kevin Cowtan.

- (5) In making this offer, WG1 explicitly accepted that honouring this commitment in 4.6 years time could lead to other projects being cancelled.
- (6) WG1 therefore binds any future CCP4 Executive to honour the commitment to Kevin, except and unless CCP4 has collapsed.
- (7) WG1 required the Chair to notify York of this decision and to confirm with Kevin that York will now guarantee Kevin a permanent underwritten position.

Kevin returned.

4 Managers report

1. Finance. KSW asked CB to report on the current financial status. With the usual caveats and additional uncertainty caused by moving away from the direct invoicing of companies, the balance sheet looks healthy, with an underspend predicted for this financial year (FY). This would be, as much as possible transferred to next FY, which would leave funds to fund an additional position. As yet the credit crunch has not effected the income, two companies having cancelled licenses, but two new companies being taken onto the books. KSW thanked CB for his excellent work on the finances and for overseeing the relocation packages.
2. The mechanics of the move to RAL were discussed at length together with their impact on staffing levels. A number of core staff had left or chosen not to relocate. WG1 expressed dissatisfaction that there would be a hiatus in staff levels at this crucial time. Particularly as the new grant was about to start and the need for the new GUI pressing. Whilst understanding the frustration, the Chair and Manager felt that the circumstances are such that there was no easier solution. However, they welcomed the offer from Frank Von Delft to host a GUI programmer in Oxford if such a person is appointed in advance of the research complex being completed.

KSW informed WG1 about the establishment of a number of Working Parties (WPs) which report directly to the Executive at the biannual developers meetings. A corrected list of the WPs together with their reports for the previous 6 months for the November 2008 meeting will be sent to WG1 in January 2009. Individual activity reports as in previous years were felt to be unnecessary given these WPs.

5 Elections

Member of Executive

Peter Moody was proposed by Nick Keep

Alun Ashton (absent) was proposed by Andrew Leslie

Peter left the room. After a very close vote, Peter was elected to the Executive. WG1 was pleased that two such strong candidates stood for the post. (The current Executive did not vote)

Peter returned to the room.

Chair designate

Jim Naismith left the room.

After discussion of WG1, Jim Naismith returned.

WG1 requested Jim Naismith stay for one final year to ensure handover and he thanked WG1 for their confidence and agreed.

Two candidates were proposed for Chair designate

Keith Wilson was proposed by Yvonne Jones

Martin Noble (absent) by Elspeth Garman

Keith left the room. The current chair summarised the contributions of both to the grant and to CCP4.

There was considered discussion of the strengths of the two candidates. The meeting felt both were excellent choices and either would take CCP4 forward.

The Chair did not vote but the remainder of the Executive did.

Martin Noble was elected to the post of Chair designate. WG1 felt expressed its thanks to both candidates for standing and acknowledged their contribution to CCP4 over the years.

Martin will become Chair at the January 2010 meeting.

The Executive is now

Randy Read co-opted

Garib Murshudov co-opted

Eleanor Dodson co-opted

Kevin Cowtan co-opted

Keith Wilson Manager, ex-officio

Simon Phillips elected, 1 year remaining

David Rice elected, 2 years remaining

Peter Moody, 3 years remaining

Phil Evans elected WG2, ex-officio

Martin Noble, chair designate (Jan 2010)

Jim Naismith, elected Chair WG1, 1 year remaining

6 Next Study Weekend

This will be at Nottingham again, and back to the traditional Thurs/Fri/Sat. Suggestions on topics to Phil Evans soon please.

7 AOB

There was none.

Appendix 1 Chairman's report on behalf of the Executive

1 Study weekend

We thank Randy Read and Gerard Kleywegt for organising such a successful meeting on "*Low Resolution Structure Determination and Validation*".

We look forward to this years study weekend organised by Clemens Vornrhein (Global Phasing), Arwen Pearson (Leeds) and Elspeth Garman (Oxford) on the topic "*Experimental Phasing and Radiation Damage*". The final attendance is 320

2 State of the suite

I would like to record the thanks of the entire community to the core CCP4 staff, Martyn, Charles, Ronan, Norman, Graeme, Peter & Francois. The suite continues to expand in usefulness, reliability and uptake. We currently derive an external income of approximately £882K per annum from around 130 licences. The more robust regime we implemented for monitoring the projects, where we measure progress against milestones, is bedding in. We will hold a full meeting of developers in

April (15-17th at The Cosener's House), a smaller follow up one day meeting in the autumn will review reports from the various working parties.

The release of CCP4 v6.1 is a major addition to functionality. I will highlight some specific programs below. As part of this release we have extended and overhauled our testing procedures, we are finding and fixing bugs before they go out the community.

We have said a sad goodbye to Peter Briggs, Maeri Howard and Francois Remacle this year. We were extremely sorry to see them go but we thank them for their contributions over a number of years and wish them well in their future careers.

3 BBSRC Grant

The grant was funded in full. The referees comments were glowing and we are grateful to BBSRC for their farsighted support of CCP4. As a community we need to recognise the hard work done by the people who put the grant together. The list of honour is very long but special thanks to Kevin Cowtan, Harry Powell, Andrew Leslie, Charles Ballard, Martyn Winn, Martin Noble, Randy Read, Eleanor Dodson, Peter Briggs and Phil Evans.

As Peter Briggs has left CCP4, Liz Potterton is now overseeing the GUI. More on the move to Diamond and new appointments below.

The final report on the last grant has been submitted.

4 Executive

The Executive is currently
Randy Read co-opted
Garib Murshudov co-opted
Martin Noble co-opted
Eleanor Dodson co-opted
Kevin Cowtan co-opted
Keith Wilson Manager, ex-officio
Simon Phillips elected, 1 year remaining
David Rice elected, 2 years remaining
Phil Evans elected WG2, ex-officio
Jim Naismith, elected Chair WG1, 0 years remaining

One additional elected representative is required this year.

An election is required for the new chair.

The community owes the co-opted and elected members of the Executive (Eleanor, Keith, Randy, Martin, Simon, David, Garib, Kevin and Phil) together with Martyn Winn and Charles Ballard a thank you.

5 Finances

There was no increase in the licence fee last year. The Executive suggests we consider a 5% increase for Jan 2010 to keep pace with inflation.

Keith Wilson (CCP4 manager) will present a more detailed overview of finances, posts and commitments.

The suite is financially stable, provided commercial income holds up, and we do not foresee any contraction. We are, however, acutely aware of the need to invest properly, review projects and re-jig priorities where necessary.

6 Major projects

(6.1) The graphics viewers: Paul Emsley, the author of COOT, is the first CCP4 fellow and is based at Oxford. COOT 0.5 is released and widely taken up. It includes Ramachandran refinement restraints, "fixed atoms" in refinement, chi squareds traffic lights, sequence assignment, improved key-bindings, improved NCS tools, integration of Molprobity rotamer probabilities, the move to PDB 3.x format compliance, and a restraints editor. It is already the de-facto standard in model building. Stuart McNicholas as per agreement from WG1 is now leading the development of CCP4MG. Not only is the QT (more robust code) version more stable and faster but the graphics are extremely good. The latest version has the COOT button which allows seamless transfer between the programs. The latest stable release is part of CCP4 but can also be loaded from the MG site. The QT version will be released this month (Jan 09).

(6.2) MOSFLM (and its GUI). We fund one person to work with Harry Powell (who is grant funded). Both gui and MOSFLM continue to improve significantly. The new spot finding algorithm is much more powerful. Full TESTGEN functionality has now been incorporated, plus the facility to process images as they are being collected. Almost all the functionality of ipmosflm is now available. The GUI creates a new standard in usability and reduces button pressing to a minimum, e.g. it is now possible to press one button to index, select spacegroup and calculate mosaic spread. It is now being rolled out across synchrotrons and I urge people to upload it. In the near future it will become possible to test space groups (pointless) and scale data during image integration. Corrections to handle detector corners (important in 3 x 3 detectors) in AIMLESS are being developed in collaboration between MOSFLM team and Phil Evans.

(6.3) PiMS: We currently fund two positions. The Executive will schedule and conduct (with outside help) a review of continued CCP4 support (akin to that for the MG initiative). Unlike MG, we are not the only stakeholder, thus we cannot "direct" the project entirely.

PiMS is now used by MPSI, SSPF, and the OPPF in the UK, and also IRB, ISB, and CSIRO. We are in discussion with three companies about commercial licences for PiMS. PiMS will remain free for academic use. The licences are based on the CCP4 licences.

PiMS2.2 is product grade, with a range of features covering most aspects of protein production. The benefits it provides include traceability, searchability, manageability, continuity, flexibility, and future proofing. Planned work includes completion of xtalPiMS, integration with synchrotron facilities, a hosted service, usability improvements, better construct management, better scaling for large labs, and instrument integration.

We envisage that the future of PiMS is under the INSTRUCT umbrella, and are seeking bridging funding to cover FY2010. We hope to show that PiMS the right vehicle for the BBSRC's goal of sharing experimental data, in the case of protein production. www.pims.ac.uk

(6.4) Molecular replacement: We support MrBUMP and Balbes and benefit enormously from PHASER. Plans to upgrade MrBUMP to deal with protein-protein complexes are imminent. We will explore a possible web service for this.

(6.5) Experimental phasing and model improvement: We are going to make a push to implement automated front ends (in some ways analogous to MrBUMP) to utilise the powerful software we have developed. The programs PARROT and BUCANEER (Kevin Cowtan et al.) will be introduced in version 6.1. PARROT is a new density modification program to replace DM – it is fully automated (requiring just sequence and MTZ, and optionally heavy atoms or model for NCS),

and gives substantially better results than DM without taking significantly longer to run. BUCCANEER continues to evolve; it is fast, robust and competitive over a range of resolutions, and provides best-of-class results for low resolution problems (2.8-3.6A). The version of PHASER released with 6.1 gives us new tools to calculate phases from SAD information, starting from a substructure or even a molecular replacement model.

(6.6) Refinement: The new REFMAC with refinement of twinned data is now available. Its performance suggests this is the best in the class. The procedure is fully automatic once the twin is selected and the new GUI makes this very easy. SAD refinement is close to completion. We are aware that there remain issues with low resolution for the most challenging projects. Escaping from the tyranny of anecdotes by properly evaluating performance is underway and we expect further improvements. There has been an overhaul of dictionaries, the funding of PRODRG and JLIGAND will mean more easy-to-use and robust libraries for refinement.

(6.7) New GUI: We fund Liz Potterton and she will fill the role of scoping out and designing the new GUI. There will be a series of meetings to establish what users want, how it can be delivered and on what time scale. It seems likely that we will use QT as the graphical toolkit.

(6.8) The core suite: This remains our biggest investment. The current team have worked heroically to release 6.1. We all recognise that the way we manage releases has to change, the suite has grown too large and too complex to continue to work as before. One serious problem has been fixing broken code (which might not compile on some platforms), assuming delivery of fixes and rewriting GUI's. The multiple UNIX flavours have complicated this task. New testing procedures, common program repositories and automatic nightly building are planned to lead to a more rapid release schedule. The precise model for future releases remains unclear and is being scoped out. It is a high priority to make this automatic and seamless. We are committed to an overhaul of the PDB format (when changed by the PDB) and an extension to the mtz format within the next few years.

We ask that WG1 agree to de-emphasize (with a view to discontinuing) IRIX support.

We may also come forward with proposals next year to focus on fewer LINUX flavours. Any such suggestions would be based on extensive consultation with the user community.

7 Outreach

CCP4 will continue to support workshops, both within the UK PX community and worldwide.

The Summer School was organised and run by Elspeth Garman and Martin Noble. It was a resounding success, and we send Elspeth and Martin our congratulations and thanks.

Garry Taylor and Jim Naismith will run the summer school in 2009.

Expenditure on outreach activities

South West Structural Biology	£8k
Oxford summer school	£9k
Carlisle (Northern)	£7.25k
APS	£10k
Tokyo	£15k
ACA	£5k
IUCr	£5k

8 Licence issues

None

9 Research Complex at RAL

In September Ronan Keegan and Charles Ballard will move to RAL into the Research Complex at Harwell (RCaH), which will be completed at the end of September 2009. The terms of this move have been agreed. Normal Stein will leave CCP4 around this time, having declined to move. We will advertise two new positions in the New Year to be filled at RCaH at around the September time frame. Martyn will continue to be part time (decreasing percentage) while he remains in Daresbury.

10 Other matters

The Executive will ask that a second CCP4 fellowship is created (Paul Emsley currently holds the original one). The Executive (minus Kevin Cowtan) has been in discussion with York University on issues surrounding Kevin's future involvement with CCP4 and his position at York. It seems likely that an arrangement where Kevin is offered a deferred CCP4 fellowship in 2009 to be taken up at the end of a grant (2013) will result in York giving Kevin a fully underwritten independent permanent academic position. York will agree to accept the risk that CCP4 may become insolvent between now and 2013 (or at any time thereafter). CCP4 would agree that the fellowship offer will be made in 2013, provided funds are available. Long term or large commitments require WG1 approval since in this case we propose agreeing to funding almost 10 years in the future, it must be a community decision. The Executive (minus Kevin) strongly support this proposition and recommend WG1 adopt it. The Executive feels there is a window of opportunity at present. The Chair is happy to discuss the matter with any member of WG1.

Kevin's contributions to CCP4 over the years have been substantial, including:

- Core libraries: the Clipper libraries provide the basis for COOT, CCP4MG, PARROT and BUCCANEER, and are also used in CTRUNCATE, POINTLESS, AIMLESS, ARP/wARP and a number of other projects worldwide.
- Major applications: DM, DMMULTI, FFFEAR, PROFESSS, PARROT, BUCCANEER
- Minor applications: MAPMASK, NCSMASK, CFFT, CINVFFT, CSFCALC, CPATTERSON, CHLTOFOM, CSIGMAA, CPHASECOMBINE, CPHASEMATCH, CANISO, CECALC, CSEQUINS, CSYMMATCH, CONVERT2MTZ
- Program output: Initial author of JLogGraph inline graph viewer, contributor to the BAUBLES program output annotation tool.
- Documentation: Creator of and principal contributor to the ccp4wiki.org documentation project.
- Teaching and outreach: Outstanding regular tutor at CCP4 and other workshops, teaching a range of CCP4 software.
- Funding: Major contributor to the 2008 CCP4 grant renewal.

CCP4 Working Party reports Nov 2008

WORKING PARTY 0: Core activities
COORDINATOR: Keith Wilson (KW)
OTHER CONTRIBUTORS: Martyn Winn (MDW), Peter Briggs (PB), Charles Ballard (CB), Francois Remacle (FR), Ronan Keegan (RK) and Norman Stein (NS)
MARCH - NOVEMBER 2008 <ul style="list-style-type: none">• Releases How much achieved:<ul style="list-style-type: none">• Get 6.1 out asap. To be the last monolithic release. CLOSE.• Step back and decide exactly what we want. (whole team). TO BE DONE.• Aim for package releases. Establish system for automated release of individual modules as they are updated. Coordinate with developers. (core team + developers) 6-monthly announcement of latest contents. How to identify set of versions in a given snapshot. Action: Plan what the packages are, especially what goes into the core packages. (MW to lead). REVISIT NOV08.• Survey other software projects of comparable size (MW) NOT DONE.• Automatically inform users when new versions are available. (FR) FR LEFT.• Coordinate between packages which have inter-dependencies.• Regression testing: a workshop to initiate this? NOT DONE.• Developers to establish appropriate test data to simplify full testing on platforms by the core team and effectively devolve some of these onerous tasks from the core to the developers. (PE proposal) IN HAND. GW has started acquiring data• AA requested email list for system admins, tools for addressing a multi-user shared environment, and an approach to exploiting big computers (and multi-core desktops) NOT DONE• Core staff:<ul style="list-style-type: none">○ Recruit replacements for Peter and Maeri asap. These posts should be based at Rutherford, but conflict with continuity of experience and induction to the team. DELAY OF MOVE○ Peter replacement to work on the GUI/database with Liz as required by the grant. Should have this person in place in October. FR first choice, but left CCP4. This is on hold till relocation.○ Recruit MH replacement to lower finance and admin load on Charles. Spending much too much time on finance details at present. OCT 09 IN RUTHERFORD○ Continue to monitor times on the various areas over a longer period (MW to coordinate). ABANDONED○ Revisit Martyn's questions about whether some aspects of support can be dropped. This may be helped by the Wiki developments. IN PROGRESS• Research activities of core team:<ul style="list-style-type: none">○ Vital that core team have some time to devote to research and development.○ Need to be flexible wrt to the projects on which research staff are focused, not just continue with the status quo. Need a consensus with core team○ Review areas of research for the team. (KSW) NOT DONE GIVEN LOSS OF STAFF• Relocation: DELAYED UNTIL OCT 2009<ul style="list-style-type: none">○ Research complex to house CCP4 at Rutherford. Completion date late 2009.○ CBB and RK to relocate Sept/Oct 2009.○ PB and FR resigned. NS elected not to move, but appointed 1 more year.

WORKING PARTY 1: Program output, Manual & WIKI, Publicity Material
COORDINATOR: Martyn Winn (MDW)
OTHER CONTRIBUTORS: Kevin Cowtan (KC), Phil Evans (PRE), Eleanor Dodson (EJD), Graeme Winter (GW)
ACTIVITIES April 08 TO PRESENT <ul style="list-style-type: none">• General:<ul style="list-style-type: none">○ MDW has taken over as coordinator of WP1• Baubles/Program Output:<ul style="list-style-type: none">○ PJB has documented Baubles at http://www.ccp4.ac.uk/group/documents/pjb_projects.php○ Baubles incorporated into main CCP4 and included in CCP4i for test releases 6.0.99a onwards (ccp4i: "View Annotated Log in Web Browser")○ Baubelised programs: buccaneer, parrot, scala, pointless, phaser (latest version, not in current release)○ GW polled ccp4-dev on programs to update (1 response)• Loggraph:<ul style="list-style-type: none">○ FR wrote new Java version "JLogView" which can run as standalone application or as applet.○ Finished but not yet in test release series.○ FR drew up a draft new loggraph markup specification (new_markup.doc). Available on internal pages - not sure if circulated.• Wiki:<ul style="list-style-type: none">○ Up and running○ KC has provided regular summaries of contributions.• Manual:<ul style="list-style-type: none">○ Looked at by MDW. Summary to be presented in Nov 08 talk.

WORKING PARTY 2: Data Processing
COORDINATOR: Andrew Leslie
OTHER CONTRIBUTORS: Phil Evans, Harry Powell, Luke Kontogiannis, Gwyndaf Evans, Wes Armour, Norman Stein, Graeme Winter
<p>ACTIVITIES MARCH-NOVEMBER 2008</p> <p>These are reported against the plans set in March 2008</p> <p>Andrew Leslie</p> <ul style="list-style-type: none"> • Complete tests on database of indexing images to determine optimal indexing parameters. DONE • Check current algorithms for determining reduced cell. POSTPONED. • Finish local background spot finding algorithm. DONE • In addition: 1. Built in more intelligence into spot selection for autoindexing, to avoid noise/ice spots for weak diffraction, reduce threshold for weak images. 2. Assembled 16 datasets for regression testing of ipmosflm, devising criteria for pass/failure. 3. Initiated investigation of corner effects in tiled CCDs. <p>Phil Evans</p> <ul style="list-style-type: none"> • Pointless and SCALA: bug fixes, respond to complaints, no major developments. DONE. Specifically, improvement of optimisation of SD correction parameters, improved outlier filtering for anomalous correlation coefficients, fix bugs in handling of reflections flagged by MOSFLM as having problems, several minor POINTLESS bugs fixed. • AIMLESS: Rewrite of SCALA to allow more flexibility, new scale models, better analysis, assessment of data, advice to user eg automatic optimisation of resolution limits, radiation damage vs completeness etc. Significant progress, will now determine scales and write statistics. <p>Harry Powell</p> <p>(i) iMosflm</p> <ul style="list-style-type: none"> • Implementing necessary changes in ipmosflm (eg new XML) to allow implementation of WAIT for new images, non-zero twotheta angles, XML for automatic backstop shadow determination. DONE <p>(ii) Mosflm</p> <ul style="list-style-type: none"> • Complete the implementation of Bruker detectors, 1 byte-per-pixel images DONE • Finish off multi-circle goniostat code DONE • Implement spatial distortion and obliquity corrections for Pilatus detectors. NO LONGER REQUIRED • Extend backstop shadow detection to rectangular backstops and allow for support arm. NOT FINISHED • Generate artificial test data for investigation of effect of mosaicity on success of autoindexing. DONE • Allow launch of imosflm from CCP4i GUI. DONE (By Peter Briggs) • In addition: Debugging, investigating feasibility of parallelising code, improved build procedures, partial rewrite of JPEG routines. <p>Luke Kontogiannis</p> <ul style="list-style-type: none"> • ~30 known bugs left to fix. MOST SERIOUS FIXED, SEVERAL REMAIN. • Complete full implementation of TESTGEN, WAIT (for new images), non-zero two-theta images, automatic backstop determination. ALL DONE. • Feature par with ipmosflm, giving release version 1.0. RELEASED. • Allow submission of Pointless and SCALA jobs from GUI. DONE. • In addition: Introduce many more parameters. Allow chained spot finding, indexing and mosaicity estimation. Improved error messages associated with indexing. <p>Leslie and Powell</p> <ul style="list-style-type: none"> • Wiki documentation for imosflm/ipmosflm. VERY LIMITED • Regression testing. PARTIAL TEST SUITE IN PLACE, REQUIRES EXPANSION • Options for parallelising code. SOME PRELIMINARY WORK <p>Wes Armour & Gwyndaf Evans</p> <ul style="list-style-type: none"> • Extend numerical methods to handle partially illuminated volumes 75% DONE • Incorporation of analytical methods to reduce memory and cpu requirements. DONE • Use small molecule crystals as a test system. AWAITING BEAMTIME • In Addition: Analysed tomographic data collected at SLS. Demonstrated that reasonable quality reconstructions can be obtained even from poor quality raw data. <p>Francois Remacle LEFT CCP4, NO REPORT</p> <ul style="list-style-type: none"> • Develop reliable detector gain estimation function • Support additional detector types (Mar555) • Improve backstop masking function

- Develop new features for the image viewer.

Graeme Winter

- Finish release of 0.3.0 to go with CCP4 6.1. NOT YET READY, BUT PREVIOUS VERSION WILL BE DISTRIBUTED WITH CCP4 6.1
- Complete implementation of "Chef" to make automatic decisions about optimum resolution limits, best anomalous/dispersive differences. REALISED THAT THIS NEEDS TO BE ADDRESSED AT THE INTEGRATION STAGE (RATHER THAN SCALING/MERGING), INVESTIGATION ONGOING.

Norman Stein

- First principles twinning calculation (in collaboration with PRE). DONE. USES LEBEDEV'S CODE FROM SFCHECK
- Attempt to quantify the effects of translational NCS. NOT DONE
- Work with unmerged data. NOT DONE
- Handle multiple datasets in a single MTZ file. NOT DONE
- In addition: Use intensities for anisotropy calculation. Fixed bug in DANO column. Changes to column labels.

WORKING PARTY 3: Experimental Phasing

COORDINATOR: Paul Emsley

OTHER CONTRIBUTORS: Randy Read, Airlie McCoy, Raj Pannu, Pavol Skubak

ACTIVITIES MARCH 2008 TO PRESENT

* Phaser:

Improved SAD phasing, NCS handling
Parallelization, Improved Baublization(?)

Crank, BP3, Refmac:

Log files for Baubles
Window version works up to density modification

- basic Refmac multivariate SIRAS phasing implementation with promising preliminary results.
- basic Bp3 multivariate SIRAS phasing implementation (currently attempting to reproduce Refmac results).
- baubles compliant Crank implemented (version 1.3.0)
- implementation of Parrot and massive tests performed Parrot->Buccaneer.
- buccaneer+SAD integration with successful massive tests (but, no comparisons with other functions). (Buccaneer + SAD is default for Crank in ccp4 6.1 if SAD data is given.)

WORKING PARTY 4: Molecular replacement
COORDINATOR: Garib N Murshudov
OTHER CONTRIBUTORS: Airlie McCoy, Randy Read, Martyn Winn, Ronan Keegan, Alexei Vagin, Fei Long, Andrey Lebedev, Paul Young
ACTIVITIES MARCH 2008 TO PRESENT (HALF A PAGE) Phaser: Amongst developments in MR are *automatic determination of search order *refinement of search model overall B-factors *improved minimization Molrep: Pseudo-translation option has been improved Molrep has been made ready for massive tests of many translation function peaks with reftmac ZANUDA – automatic check and correction of space group program has been implemented (by Andrey Lebedev). MrBump: 1. It is incorporated into the CCP4 6.1 release 2. It makes use of the CCP4 database handler for tracking job information. The underlying jobs carried out by Mrbump can be viewed as sub-jobs in the CCP4db graphical viewer. This allows proper integration with CCP4i and the project view provided by the CCP4db graphical viewer. 3. Improved output in the log file. A brief summary of the current set of results is given after the completion of each search model's processing. 4. Currently working on incorporating Buccaneer/Parrot. 5. We're looking at improving the template model search, perhaps making use of search tools such as HHpred BALBES: Check all allowed space groups On the webserver version link has been added to automatic model building – ARP/wARP ZANUDA was made available via webserver It is ready for ccp4 release Regular update and tests of pdb entries Selection of twinned and pseudo-translational cases from pdb

WORKING PARTY 5: Model building, refinement, and ligands
COORDINATOR: Kevin Cowtan
OTHER CONTRIBUTORS: Garib Murshudov, Paul Emsley, Raj Pannu, Serge Cohen
ACTIVITIES MARCH 2008 TO PRESENT A group of WP5 developer met on the 6 th August 2008. Productive discussions were held, summarized below. No new initiatives were launched during the meeting itself, however the exercise was useful in keeping all of us in touch with what the others are working on and what challenges they are facing. Murshudov group: <ul style="list-style-type: none">- release twinning code for 6.1- integrate and release SAD function for 6.1- reftmac minimiser stability improvements- development and release of JLigand Cowtan group: <ul style="list-style-type: none">- Write and release parrot: automated, improved replacement for 'dm'- Improve buccaneer output: numbering, side chains- Improve buccaneer performance: optimisation, fast mode, threading- Backport clipper, parrot, buccaneer for inclusion in CCP4 6.1 Leiden group: <ul style="list-style-type: none">- Refmac SAD function improvements: anisotropic ATPs, simultaneous B and anom occupancy refinement, robustness (massive tests)- basic Refmac multivariate SIRAS function implementation for both refinement and phasing- preliminary implementation of function for joint refinement of protein and ligand- basic Bucaneer+SAD integration with successful massive tests

WORKING PARTY 6: GUI and graphics
COORDINATOR: Martin Noble
OTHER CONTRIBUTORS: Peter Briggs, Liz Potterton, Stuart McNicholas, Paul Emsley, Bernhard Lohkamp, Daan van Aalten, Alex Schuttelkopf
ACTIVITIES MARCH 2008 TO PRESENT LP and SM Most major functionality ported to QT. Improvements in functionality including atom selection, movies and picture wizard. Build and distribution system improved and number of Linux distributions minimised DvA and AS: PRODRG into CCP4 All atom representation (1 mo): done - CIF topologies now contain explicit hydrogens. SMILES input (1 mo): done, using (a)polar hydrogens as determined by PRODRG Coordinate generation with REFMAC (1 mo): this turns out to be a major hurdle. REFMAC does not appear to have a sufficient radius of convergence when used as a simple minimizer. Our workaround is to improve the accuracy of the internal (distance-based) coordinate generator as a prequel to REFMAC - but this is likely to cost 1-2 months more than planned. Building/interfaces with GUI (2 mo): discussions have taken place and it has been decided that JLigand will be used as the graphical interface for drawing molecules as input for PRODRG.

WORKING PARTY 7: PIMS

COORDINATOR: Chris Morris

OTHER CONTRIBUTORS:

Bill Lin

ACTIVITIES MARCH 2008 TO PRESENT

Work on xtalPIMS, which is now in use at OPPF. Designing user experience, and beginning to implement the new design.

Adopted by IRB, ISB, and CSIRO. Discussions with three companies about commercial licences for PiMS. PiMS will remain free for academic use. The licences are based on the CCP4 licences.

PiMS2.2 is product grade, with a range of features covering most aspects of protein production. The benefits it provides include traceability, searchability, manageability, continuity, flexibility, and future proofing.