

## **CCP4 Working Group 1**

Great Woodhouse Room, Leeds University  
Friday 4 Jan. 2008.

Present.

Jim Naismith (St. Andrews – Chair)  
Keith Wilson (York - Secretary)  
Lindsay Sawyer (Edinburgh)  
Peter Artymiuk (Sheffield)  
David Rice (Sheffield)  
Phil Evans (MRC-LMB)  
John Helliwell (Manchester)  
Jenifer Littlechild (Exeter)  
Leo Brady (Bristol)  
Elspeth Garman (Oxford)  
Ian Tickle (Astex Technologies)  
Simon Phillips (Leeds)  
Andrea Hadfield (Bristol)  
Vilmos Fulop (Warwick)  
Peter Moody (Leicester)  
Kate Brown (Imperial)

Nicholas Keep (Birkbeck)  
Richard Paupit (AstraZeneca)  
Mark Banfield (Newcastle)  
Jim Spencer (Bristol)  
Thomas Sørensen (DLS)  
Adrian Lapthorn (Glasgow)  
Stephen Prince (Manchester)  
Tadeusz Skarzynski (GSK)  
Katherine McAuley (DLS)  
Alun Ashton (DLS)  
Mark Roe (ICR)  
Eleanor Dodson (York)  
Garib Murshudov (York)  
Robert Esnouf (Oxford)  
Andrew Leslie (MRC-LMB)  
Charles Ballard (STFC - minutes)

Apologies.

Martyn Winn (STFC)  
Randy Read (Cambridge)  
Dave Stuart (Oxford)

Neil Isaacs (Glasgow)  
Kevin Cowtan (York)

Presented Documents.

- i. Chair's Report
- ii. Financial Report
- iii. Core Group Relocation Report
- iv. Working Party Reports (0-5,7,8)

### **Previous minutes**

Previous minutes accepted.

### **Matters Arising.**

No issues raised.

### **Chair's Report (Jim Naismith, see attached)**

The Chair thanked Garib Murshudov and Frank von Delft for their efforts in organising the 2007 Study Weekend on Molecular Replacement, and Randy Read and Gerard Kleywegt for the organisation of the 2008 Study Weekend on Low Resolution

Structures and Validation. The attendance for the 2008 Study Weekend was given as 440, which is in line with previous years despite the increase in charges.

The Chair's Report outlined the current commercial activity and the progress in the Grant renewal application. It is expected that the result of the application will be known in March 2008. The Chair thanked Martin Noble, Randy Read, Simon Phillips, Kevin Cowtan, Keith Wilson, Martyn Winn, Peter Briggs and Eleanor Dodson for getting the grant into good shape.

The meeting was informed of an agreement with Richard Blake (Computational Science and Engineering Department head) to charge pFEC at 80% on core contracts and new contracts at STFC. CCP4 expects a similar FEC level to be applied in contracts with Universities and Institutes.

The results of a review by the CCP4 Executive on molecular graphics programs within CCP4 were briefly presented. This determined that merging COOT and CCP4MG was not at this point advisable, but that greater interoperability be targeted. The Executive recommended that the future level of funding be reduced to 1 FTE, to maintain and develop CCP4MG. This was agreed by the meeting.

Progress in iMosflm and PiMS developments was outlined. The ease of running iMosflm/Moslfm on the windows platform was considered to be a major improvement in functionality. The question of the status of PiMS was raised by Phil Evans. He asked whether PiMS was at a suitable level of usability to be used in non-partner laboratories, and how work was proceeding on supporting a range of robotic crystallisation systems. Keith Wilson and Rob Esnouf indicated that over the next six months it would be important for non-partner laboratories to try PiMS. Further, that the high throughput support was reasonable, but the standalone procedure support needed work. The XtalPiMS development at Oxford (OPPF) was addressing many of the issues in robotics support. With regard to iMosflm and other applications in the suite Eleanor Dodson requested better notification and support of updates, as many users are using out of date versions of programs. Charles Ballard indicated that this would be addressed to a limited extent within the planned 6.1 release, with a notification of updates included within the CCP4i. This work was considered to be of the highest priority. The chair committed to deliver this functionality this year.

The CCP4 Executive, as part of the graphics program review, had noted the increased requirements for the GUI/database/results presentation effort. It was proposed that 1 FTE (in addition to the Grant post) be earmarked for this. This was agreed by the meeting.

The Chair proceeded to cover the license/GPLv3/GGP4 issues and the proposed relocation of core staff to the Research Complex at RAL (see document). The difficulties that have occurred in getting the relocation packages offered to staff were outlined. Simon Phillips is the first Director of the new RAL research complex, the meeting offered its congratulations to him. It is to be hoped that the "pull" that Simon can exert will help.

## **Election to Executive Committee.**

David Rice was proposed by Simon Philips and duly elected to serve a three year term. The meeting offered its congratulations.

The Chair reminded all present that his term ends Jan 09. Nominations are open, they can be made before or at the next meeting. There is also a slot for a new elected member of the executive.

## **Managers Report** (Keith Wilson, see also Finance Report and WP reports).

*Finances (Charles Ballard):* There are various complications including the outstanding liabilities (£82k older than 12 months), and unknowns regarding the rate of payment of proforma invoices, and the grant. For FY 07/08 the listed underspend is £96k, this is partially due to the 28 months of delays in recruiting staff (£140k). For FY 07/08 there are approximately £120k of proforma invoices outstanding. This income can only be booked when payment is received. The current income estimate of £820k assumes £60k non-payment. It is also estimated that a further £50k (in addition to the £35k currently written off) will be written off for historical non-payment of invoices. Advance spending on workshops should reduce the underspend to near zero, while adding flexibility to FY 08/09. FY 08/09 income figures assume £60k in income is delayed. It is estimated that there will be 2.5-3 open positions in FY 09/10. The meeting accepted and understood the difficulty in zeroing out the budget each year, essentially a requirement of STFC. A cautious budget always ends up underspending, yet a deficit will not be tolerated. Overall, the Executive suggested we do not pencil any new increases in licence fee, the meeting agreed.

*Study Weekend:* The meeting thanked the STFC and Leeds staff, Maeri Howard, Shirley Miller, Damian Jones, Nina Woodall, Laura Johnstone, Tracey Kelly, Stuart Eyres, and Bev for their efforts.

*Management:* It has become clear that given the size of CCP4 a more formal process of management and reporting is required if we are to continue to justify to our funders and stakeholders value for money. The Executive has established Working Parties, which are to monitor and lead developments in key areas, reporting on a six monthly basis (March and September).

## **Any Other Business.**

Request for suggestions of topic for the next Study Weekend, to be held 3-5 Jan 2009 in Nottingham. Suggestions made (can other suggestions be e-mailed to Phil Evans):

- a. CCP4 overview (Keith Wilson)
- b. Automation Decision Making (Tadeusz Skarzynski)
- c. Experimental Phasing
- d. Co-factors and Ligands (Rob Esnouf)

The meeting closed with the Chair thanking all present for attending.

## **Appendix 1 Chairman's report on behalf of the Executive**

### **1 Study weekend**

We thank Frank von Delft (SGC, Oxford) and Garib Murshudov (York) for organising a very exciting program for last year.

This year we all look forward to "*Low Resolution Structure Determination and Validation*", and thank the scientific organisers Randy Read and Gerard Kleywegt

The final attendance is XXX

### **2 State of the suite**

I would like to record the thanks of the entire community to the core CCP4 staff, Martyn, Pete, Charles, Francois, Ronan and Maeri. The suite continues to expand in usefulness, reliability and uptake. We currently derive around £800K per annum from around 130 licences. We have instituted a more robust measurement regime for all projects that we fund. This has introduced milestones for the first time.

### **3 Grant**

The renewal was submitted on time. We went through a 2 stage process, outline and full. The feedback on outline was very good. The final proposal was circulated to WG1, but is attached again. There were four themes. We await the result.

### **4 Executive**

The Exec 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  
Simon Philips elected  
Phil Evans elected WG2  
Jim Naismith, elected Chair

The community owes the people on the Exec a huge vote of thanks, I include Martyn Winn, Charles Ballard and Peter Briggs.

### **5 Finances**

Keith will present a detailed update on our position. In summary the Exec think we are financially stable, we have better data on the implications of FEC. If the grant is refunded we do not have to contract our efforts. A number of projects will end over the next few years. We cannot take on more activity but we can re-direct activity as projects end.

The increases in licence fee have been well judged. For the moment we do not propose to increase the fee beyond already agreed rises.

### **6 Major projects**

The graphics viewers: Paul Emsley, the author of COOT, is the first CCP4 fellow and is based at Oxford.

We held a review of molecular graphics with both Exec and STAB, assisted by David Brown. This was a very positive meeting, CCP4mg has matured into an excellent tool for making figures and examining structures. On PC's the program is very stable and fast. A change to Qt over the next few months will make the program robust for MACs. Paul and the CCP4mg team (Liz Potterton & Stuart McNicholas) have worked hard to make COOT and CCP4mg viewer interoperable. Over the next year, we will see this behaviour enhanced. Going forward, we are minded to appoint one person (not two) to work with Kevin and Paul to develop MG and assist with the COOT CCP4mg interoperability. We seek WG1 permission to decrease effort on MG viewer recognising it has reached version 1 stability.

The new MOSFLM GUI continues to improve. The newest version is another huge advance. At a users meeting a list of wishes / targets were set for MOSFLM. Andrew and Harry have set themselves these goals, in 3 months we can review progress.

PIMS: PIMS version 1 has been released. BBSRC renewed funding for the full five years. We await with interest future developments.

We have begun work on a new GUI and database. Pete Briggs work is fantastic and very exciting. I suggest you have a look if you get the chance. We propose to invest in GUI development by moving a person full time to this.

## 7 Outreach

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

The St Andrews workshop was run by Garry Taylor and Jim Naismith, the students liked it. CCP4 thanks all the lecturers and in particular Garry. From CCP4, Liz Potterton had 40 students working away on the viewer. Harry Powell with the students processed a full data set in 4 minutes. A big innovation was each student had a laptop for the entire meeting and a memory stick with all lectures, data etc.

## 8 Licence issues

We reached an agreement with PHENIX. However, there remain problems. The issue is over the libraries, this has resulted in gpp4, a direct fork of the libraries. Once again, discussions have opened with Linda Baines. We have strong support from the science part of STFC (Paul Sherwood), I think we can put this to bed by releasing the libraries under LGPL version 3.

## 9 Relocation to Rutherford Lab

Simon's appointment as Director of the Research Complex should help.