

## Working Group 1 meeting

Location: Wordsley Room, Leeds University

Date: 9:30 am, Friday 6 January 2006

### Present:

J. Naismith, St. Andrews (Chair)  
P. Evans, MRC Cambridge  
K. Wilson, York  
E. Dodson, York  
N. Isaacs, Glasgow  
E. Garman, Oxford  
K. McCauley, Diamond Light Source  
M. Roe, Institute of Cancer Research  
M. Baker, Bath  
N. Keep, Birkbeck  
P. Moody, Leicester  
K. Brown, Imperial College  
M. Noble, Oxford  
T. Skarzynski, GlaxoSmithKline  
I. Tickle, Astex  
S. Phillips, Leeds  
L. Brady, Bristol  
D. Brown, Pfizer  
R. Read, Cambridge  
F. von Delft, Oxford  
C. Nave, CCLRC  
B. Luisi, Cambridge  
S. Prince, Manchester  
L. Sawyer, Edinburgh  
D. Rice, Sheffield  
T. Sorensen, Diamond Light Source  
V. Fulop, Warwick  
A. Laphorn, Glasgow  
P. Artymiuk, Sheffield  
R. Paupit, Astrazeneca  
J. Helliwell, Manchester

### Agenda:

1. Minutes for previous meeting
2. Matters arising
3. Chair's report (J. Naismith)
4. Financial report (K. Wilson)
5. Elections to executive

6. Next study weekend
7. 7 AOB

1. Minutes of previous meeting

The minutes of the last meeting were circulated and posted on the web since February. No comments have been received. The minutes were accepted.

2. Matters arising

No matters arising, not dealt with elsewhere.

3. Chair's report

The full chair's report is appended as appendix 1 and is not re-iterated here.

The meeting expressed its thanks and appreciation to Gwyndaf Evans and Martin Walsh for organising a superb meeting last year.

WG1 looked forward to an exciting meeting and thanked Tadeusz Skarzynski , Airlie McCoy and Eugene Krissinel.

The meeting was informed that there are 555 attendees registered for the meeting, the largest number for a CCP4 meeting yet. This means that the meeting will be more expensive than expected.

WG1 gave a vote of thanks to the core CCP4 team at DL. In doing so they noted the success of V6. WG1 realise the core team work behind the scenes and often only receive complaints but WG1 assured the team that the whole community values their work.

### 3.4 elections of executive members and chairman

Executive committee is listed below.

- J. Naismith (Chair, elected)
- P. Evans (ex-officio, elected WG2 Chair)
- R. Read (co-opted)
- M. Noble (elected, term complete)
- G. Murshudov (elected, term complete)
- D. Harding (ex-officio, BBSRC)
- C. Nave (ex-officio, CCLRC line manager)
- K. Wilson (ex-officio, manager)
- E. Dodson (co-opted)

The elected positions of Garib Murshudov and Martin Noble have completed their two year terms, and the positions are up for re-election. The Chair pointed out that CCP4 has grown in size and now supports a significant number of external projects. The Chair expressed concern that Exec members terms should not be automatically renewed, and should not nominate itself as this can lead to perceptions of cronyism. In particular he worried whether the community would feel comfortable with an unchanged Exec for a further three years. Simon Phillips noted that Research Councils refresh their panels for precisely this reason. WG1 felt the Exec should have a broad enough representation to avoid one lab becoming dominant.

The Chair's term ends Jan 2007 with an election for a new chair. The next chair term is for 5 years and is timed to match the length of grant. The Chair's major responsibility is the writing of the BBSRC grant proposal. Debbie Harding (BBSRC) has advised us to target a Sept 07 submission, although in practise a Jan 08 submission would be possible for funding to continue from Oct 08. The election is due to occur in January '07. David Rice expressed concern that the mechanism for appointing the chairman did not allow for an overlap between the incoming and retiring Chair. Should the schedule be altered so that the Chair has been in place for at least a year before taking responsibility for the grant? The Chair reminded the meeting that the normal route was for a future chair to join the Executive to familiarise themselves with CCP4. He stressed there were two vacancies open up this year. Failing election, the chair said the Exec would co-opt anyone who expresses an interest in being chair. It is considered desirable that the future Chair take joins the executive at least 12 months before taking over. However, it is appreciated that this may not be possible.

**ACTION:** The Executive undertook to consider whether the elections are appropriately timed. They will make suggestions to WG1 in due course.

Peter Moody requested more ongoing feedback from the executive during the year. Keith Wilson pointed out that the meeting notes were archived on the website.

**ACTION:** The Chair will circulate a mid year update to WG1, all Exec minutes will be circulated to WG1 and posted.

### 3.5 finances.

Currently growing the revenue stream, will write-off ~£70k as are unable to reduce surplus at a sufficient rate. The reduction of the surplus has been agreed with CCLRC and is connected to the winding down of the SR Department and the transfer of staff to CSED. The write-off is an unavoidable problem, which occurs as a result of changes within CCLRC and the requirements of a budgeting process which requires cautious assumptions about income and aggressive assumptions about expenditure. pFEC will have an adverse effect on finances in future.

There is in no agreement in place with CSED at this moment. The Chair and Keith Wilson will soon have a meeting with Paul Durham and Colin Nave (CCLRC) to discuss a memorandum of understanding for future finances.

John Helliwell wondered of the strange position of punishing a successful technology transfer by forcing it to run on an April to April budget. The meeting shared his concern but in the end, WG1 recognises that CCLRC has been a good home for CCP4, and that £70k over 25 years was not a bad bill for all the hidden benefits we received and hoped to receive in the future.

Clarification of point in Chair's report. The expression of the transfer from SRD to CSE not being handled well was aimed at the chair who dropped the ball. The transfer proceeded quicker than expected.

The Exec requested permission to increase the license fee in FY 07/08 (This is essentially an inflation increase as it would not occur until 2007). The Industrial reps were asked whether they would prefer a single increase of £1000 in one go, or two lots of £500. A single increase was preferred, the second site fee will be increased pro-rata.

ACTION: increase fee for 2007

The position of the executive regarding pFEC was outlined. CCP4 has currently no clear understanding of it's effect, bar that it will lead to an increase in costs. The Exec would prefer to offer 46% overheads on funded positions, until pFEC is applied to CCP4 (the renewal of the grant). General discussion supported and the meeting forbid the Exec from deviating from this position, even at the cost of loosing contracts with Universities. CCLRC have indicated they will not apply pFEC to CCP4 so long as Universities do not. Early application of FEC would seriously disrupt CCP4.

Ian Tickle requested that smaller biotechs be involved in the discussions on FEC and the effect on license costs.

ACTION: The chair will liaise with Ian Tickle to meet with and explain the consequences of pFEC to smaller companies.

### 3.6 Major projects

Paul Emsley will be funded on a CCP4 fellowship from this year (start date still be negotiated with York). The funding is not attached to any projects, and is mobile. The PE proposal was externally reviewed and found to be of high scientific merit.

The Chair asked that people who found problems with mosflm contact Harry Powell with the data. CCP4 has significantly invested in this and several labs publicly criticise the performance of MOSFLM without ever supplying data to Harry. This was recognised to

be unhelpful. Keith Wilson stated the desire of CCP4 core staff, and associated projects, to visit university and industry sites to install software and discuss development in the suite.

Peter Moody congratulated the staff on the updated and easier installation procedure. Eleanor Dodson made special thanks to Francois Remacle. A desire was expressed for some form of auto-update.

ACTION: CCP4 to investigate methods of auto updating.

Peter Moody, David Brown and Frank von Delft requested guidance on the functionality of COOT vs. MG be made apparent to users. WG1 was pleased to note that Coot will be distributed with CCP4. The chair explained it is difficult to advise users which program to use for what. Both programs are very powerful and difference users have different preferences.

### 3.7 Outreach.

WG1 thanked Garry Taylor and Jim Naismith for CCP4 summer school in St Andrews.

WG1 thanked to Murthy, Gopal and their groups for their hard work acting a local organisers for the Bangalore workshop. It was exciting and educational for all the participants.

WG1 expressed the opinion that CCP4 should promote CCP4 in China and India. The chair reminded WG1 that we have the David Blow fellowships and are very willing to support meetings.

CCP4 is progressing the organisation of a workshop in China this year, associated with the ISGO meeting.

### 3.8 Diamond

The research hotel is approved. Space is set aside for CCP4. This means that one of the three tests for CCP4 relocating has been met. All CCP4 staff have been advised that the three year clock has started, in that we expect the move to begin in 2008.

- a. construction of research complex
- b. financially doable
- c. will not destroy the suite

the research complex is being solely managed by CCLRC, therefore any move would be as part of the organisation. The research complex is due for completion in 08.

### 3.9 License

So far CLCRC has paid for CCP4's legal advice on the license. From now on it is expected that CCP4 will have to shoulder the costs.

#### 4. Financial report

Keith Wilson gave the financial report.

WG1 noted with satisfaction the continuing increase in commercial income.

#### 5. Elections.

WG1 thanked Martin Noble and Garib Murshudov for their hard work on behalf of the whole community. The chair gave personal thanks to both, and to the other Exec members for their support and efforts. This sentiment was reflected by the whole meeting. The efforts of Colin Nave, Eleanor Dodson, Phil Evans and Randy Read on our behalf are appreciated.

MOTION: Martin Noble nominated by Nicholas Keep. Elected

MOTION: Garib Murshudov nominated by Neil Isaacs. Elected

#### 6. Study Weekend

The next study weekend will be held in Reading. Ideas should be sent to P. Evans.

#### 7. AOB

WG1 congratulated Phil Evans on his election to the Royal Society.