Minutes of WG1 meeting. January 2010

The WG1 Meeting was held at 9:00-10:45 on Thursday 7 January 2010 in Conference Suite 3A/B in the Nottingham Conference Cetnre

Present

Jim Naismith (St. Andrews - outgoing Chair)
Martin Noble (Oxford - Chair)
Keith Wilson (York)
Charles Ballard (STFC - minutes)
Martyn Winn (STFC)
Eugene Krissinel (STFC)
Lindsay Sawyer (Edinburgh)
Phil Evans (MRC-LMB)
John Helliwell (Manchester)
Leo Brady (Bristol)
Frank von Delft (SGC)
Neil Issacs (Glasgow)
Vilmos Fulop (Warwick)
Peter Moody (Leicester)
Kate Brown (Imperial)
Nicholas Keep (Birkbeck)
Richard Pauptit (AstraZeneca)
Kevin Cowtan (York)
Mark Roe (ICR)
Eleanor Dodson (York)
Andrew Leslie (MRC-LMB)
Arwen Pearson (Leeds)
David Brown (Pfizer)

This list may be incomplete. The attendance list was mislaid.

Apologies David Rice, Simon Philips, Dave Stuart

1. Minutes of previous meeting

The minutes of the previous meeting were excepted. These had been circulated the previous January and are available on the web (http://www.ccp4.ac.uk/wg1).

2. Matters arising

None.

3. Chair's report (J. Naismith, see Appendix 1)

The meeting recorded thanks to Elspeth Garman (Oxford), Clemens Vonrhein (Global Phasing) and Arwen Pearson (Leeds) for organising a successful and interesting meeting last year.

The meeting recorded thanks to Keith Wilson (York), Kevin Cowtan (York), and Paul Emsley (Oxford) for organising the present meeting, which had 380 registrations.   Thanks also to Shirley Miller, Laura Johnson and Damian Jones for their help with the organisation.

The meeting recorded thanks to the organisers of CCP4 sponsored workshops throughout the last year, Garry Taylor for the BBSRC summer school [others...]

WG1 noted its thanks to the core staff; Martyn Winn, Ronan Keegan, Charles Ballard, and wished Norman Stein well in his new position. The meeting was informed of the relocation of the core team to the Harwell site, and the recruitment of 3 new positions; Eugene Krissinel (Group Leader), George Pelios (pipelines), Natalie Zhou (core).

The meeting discussed at length the relationship between CCP4 and DLS. This issue has particularly come to light given the Synchrotron Users Meeting being replaced by a DLS MX Users Meeting, and the first session (usually an introduction to CCP4) being dedicated to DLS. The Chair indicated that he had been approached by people from the ESRF who had expressed concern at this. K. Brown pointed out that STFC supported other synchrotrons as well as the DLS. R. Pauptit requested that in the future at least one ESRF speaker also be invited to the Users Meeting (please note that this is actually organised by DLS staff). The Chair expressed the belief that the partnership with DLS would make CCP4 stronger, and that the PiMS project milestones included elements that are dependent on synchrotron relationships.

The meeting expressed it's thanks to the outgoing Chair, J. Naismith. M. Noble takes over as Chair.

4. PiMS (M. Noble, see Appendix 2 for Review)

The Chair summarised the Review as recommending that CCP4 continues to contribute to PiMS with the agreement that CCP4 can distribute the software to licensees , at no additional cost, for as long as it continues to support the project, and can continue to distribute that version hereafter. The Chair recommended that the meeting agree to this and fund Chris Morris for 3 years from July 2010.

F. von Delft saught clarification on the management role of ccp4, and the IPR of the PiMS project. The Chair stated that the funding was conditional to CCP4 having a place on the PiMS board, and the continued support of the CCP4 branch by the PiMS team when PiMS was financially secure enough to no longer require CCP4 funding.

R. Pauptit stated taht the PiMS team is happy to customise PiMS for customers, but that the customers should have to pay for this. The Chair agreed that this was one model under consideration.

The meeting felt that there were benefits to the long term development of PiMS. A query from D. Brown indicated that there was very little take up of PiMS among the teams of the PIs present at WG1. F. von Delft asked why this was the case. The Chair suggested that previously PiMS had not been ready for primetime, with a clumsy user interface and difficult installation. The Chair felt these issues had now been addressed. P. Moody pointed out that the managed systems make it much easier to make the structural biology data available as required by the UK funding bodies. The meeting agreed that having this data available would have long term benefits for the community.

=> The meeting moved forward with the recommendation to fund Chris Morris.

5. Election of new Executive Member.

F. von Delft proposed by A. Leslie, seconded by R. Pauptit.

=> F. von Delft elected to serve a 3 year post.

Executive:

Martin Noble - chair
Rand Read - co-opted
Eleanor Dodson - co-opted
Garib Murshudov - co-opted
Kevin Cowtan - co-opted
Keith Wilson - ex-officio
Phil Evans - ex-officio, elected WG2 chair
David Rice - elected, 1 year remaining
Peter Moody - elected, 2 years remaining
Frank von Delft - elected, 3 years remaining

The meeting discussed changing the nomination process. The Chair stated that a call would be made and circulated to the members of WG1 in December. The nominations would then be voted on at the WG1 meeting.

6. Finances (K. Wilson)

Thanks to T. Kelly, S. Williams, J. Basnett, and K. McIntyre for their work on the Commercial liason and invoicing.

CCP4 is looking at an underspend of approx. 100k for FY 09/10. It is planned to transfer this through prepayment of workshops and deferal of income. The underspend is due to the increased payment rates from the customers, and an increase in the number of companies invoiced in the September invoice round. The grant is being used utilised.

Of note is that next FY will see the first overseas income for the group, in the form of a jointly funded position for Pavol Skubak at Leiden University.

It is planned to increase the commercial license by £500 from April 2011. This was voted on at the previous WG1 and not revisited. D. Brown suggested that every effort should be made to keep the license fee below £10k.

This years Study Weekend will make a loss of approx. £70k, this is made up of a spend of £120k and income of £50k. The meeting agreed that this was a good use of CCP4 funds. R. Pauptit suggested that CCP4 allow an exhibition. K. Brown indicated that the BSG 1-day meeting had exhibitors, so there should be no reluctance to exhibit at a 2-day meeting. N. Issacs warned that having an exhibition would fundamentally change the nature of the meeting. The Chair agreed to investigate sponsorship for elements of the event, however, E. Dodson stated that the lunchtime bytes made any sort of exhibit difficult.

Use of the underspend was discussed. R. Pauptit asked that the process of looking for projects to be sponsored be outlined. K. Wilson stated that major projects (3+ years, finance level?) go to WG1 for approval, while minor projects are passed by the Executive. As this division is arbitary R. Pauptit asked that a more formal procedure be put in place. J. Naismith said that during his term as chair he tried to take major decisions to WG1, but that CCP4 cannot be seen as a grant giving organisation as this would put it into conflict with the BBSRC. He agreed that having a the Executive make decisions without recourse to WG1 could lead to charges of favourtism, therefore, CCP4 must have a wide range of people on the Executve to provide oversight. The Chair asked the

members of WG1 to provide information on projects to Executive members, and through WG2 via it's Chair, however, the Executive require the ability to make short term decisions.

=> Chair to outline more formal procedure.

7. Working Party Reports (K. Wilson, see appendix 3)

GUI and graphics (M. Noble):

The GUI project currently has 1 post in the CCP4 grant (Greorge Pelios) and, additionally, 1 post (Liz Potterton) on CCP4 industrail money. Work has been delayed by the move to RAL and failure to fill the post in a timely manner. The GUI depends on the future direction of structure solution within CCP4. E. Krissinel, as group leader, is responsible for the overview and integration. Request for people to give input as part of User Story gathering. It is planeed to have a demo ready for the next WG1 meeting.

R. Pauptit suggeted random lab visits to see more groups working. E. Dodson said L. Potterton was looking for input.

=> Demo to be presented at next study weekend as Lunchtime byte, and to WG1.

Core Activities (K. Wilson):

The core group is looking at the release process, including the use of rsync for updates.

8. Next years study weekend.

Suggestions should be presented to P. Evans prior to the next WG2 meeting. Several suggestions were made

i. CCP4 and synchrotrons (R. Pauptit)
ii. Related technigues (L. Sawyer)
iii. Refinement and model building (J. Naismith), with validation (F. von Delft)
iv. Benchmarking (R. Pauptit)

The venue will either be Nottingham or Warwick on Wed. 5 - Fri. 7 January, 2011.

9. AOB

Several members of WG1 are not receiving the e-mails. The list needs updating.

The Chair requested that K. Wilson's contract be extended in his management role. This was felt to be important givne the relocation of the group, and the new group leader.

=> The extension of K. Wilson's position was agreed, until the end of June 2011.