Minutes of CCP4 Executive Meeting, March 2008

All members present, except DR.

Session 1 - Monday 17th March

Finance: Charles reported that the budget should balance this FY year, provided we get all invoices in, such as from SW meeting, Nottingham SW, etc. Next FY, we currently have a projected 75k underspend, after paying for Liz, Stuart, and cover for MDW. We are currently making heavy use of CSED support on admin and finance, roughly 1 FTE.

PIMS: Dave Stuart was present for this item. The BBSRC grant has 1 1/2 years to run. There are several developers at different sites, coordinated by Chris Morris as project manager and Rob Esnouf as scientist.

Jim: The CCP4 grant is probably funded in full, but no formal letter yet. Although the referees reports were excellent, the committee did voice some concerns, which we should take on board before the next renewal. There is an on-going question as to whether infrastructure should be funded through BMS. Alternatives are through individual FEC charges or as an SLA with the BBSRC. We are not keen splitting CCP4 funding into two, for support and for flagship projects.

STFC position: Martyn gave a summary of the fallout from the CSR07 settlement. There is no direct impact on CSED, but indirect effects. Peter Briggs and Maeri Howard have taken the early severance package which has been offered as part of the CSR07 down-sizing. Nina (who has been covering for Maeri recently) is also going. We should be able to get DL admin cover, at least in the short-term. More critically, we need a replacement for Pete. We will be required to consider internal candidates first.

Relocation: Staff concerned are now Charles, Ronan and Francois. It is particularly urgent for Ronan and Francois whose contracts end in October. They are unlikely to have their PITT offers before then. Can we give a provisional or short-term offer? Whether or not they agree to move depends on their role at RAL, as well as money.

Contact should be made with Simon, So Iwata and other scientists at the Research Complex. CCP4 should also decide on suitable development projects.

Licence: Linda Baines has agreed to (L)GPLv3. She has inserted her own sections 15 and 16 (as allowed in v3) which conforms to UK law. CCP4 libraries will be distributed under LGPLv3 which is implemented as a set of additional freedoms on top of GPLv3 which in turn contains the warranty and liability clauses. The new license is available now on the CCP4 web site, but the source code needs new boiler plates and the full CCP4 license needs updating to include (L)GPLv3. Paul and Kevin have agreed to use the CCP4 libraries under this license rather than gpp4. Jim will announce the new licensing on the BB.

Session 2 - Wednesday 19th March

Licence: Airlie asks if we have checked with Phenix. Phenix have a modified licence that they are happy with, but they might like to move to the new licensing.

Liz and Stuart: GUI2 has been identified as an important aim, and Pete's departure leaves a big hole. There is 1 post funded on the grant, and 1 post to be funded from industrial income. Liz will be in charge, and has circulated a proposal. Stuart is to help with Coot and GUI2, but QtMG must be properly finished. Keith proposed Liz to be funded for 3 years to work on GUI2, and Stuart for 3 years. Stuart has a proposal in preparation. It was stressed that Liz should gain requirements for GUI2 from users.

Finance: Charles has proposed a list of allowed FEC expenses for CCP4-funded positions, namely staff cost, max 2hr / week PI time, max 2hr / week local admin and computer support, 1 workstation per 3 yr, £500/yr consumables, £1000/yr travel. Kevin suggested that CCP4 developers are more demanding in computers: 1 workstation per 2 yrs, plus a laptop. The additional costs are small compared to staff costs, but the point is to have a uniformly applied list.

Relocation: Staff need to have interesting projects to work on. Francois (background in IT) should be considered for GUI2 and for the automatic updates. Martyn will discuss these with him. His DiffractionImage library is useful but he should be encouraged to take on new projects.

PRODRG: Dan presented a workplan for a FT person for 1 year. The first section covered work that would be required to include PRODRG in CCP4, such as gromacs → refmac, need GUI, interface with Coot, distribute with ccp4. Also suggestions for extras: pre-PRODRGd list, LigCheck. CCP4-core could be coordinate generation + output cif. Have enhanced product to continue to sell. Not clear how much added value. Alex funding runs out end of April.

Airlie: Randy has post on WT grant, soon. Could be contributed to HAPPy.

Session 3 - Wednesday 19th March

Jim: Eugene would be interested in CCP4 post at Rutherford. 1/3 core support, 1/3 research (he would fund), 1/3 managerial. He could be a group leader at RAL. It is a requirement that he can do research. We are interested in principle. He has UK passport.

For grant, we need to replace Pete within 6 months of grant starting.

XIA2 no change. No proposal.