

CCP4 Executive Meeting April 9th 2010

Present:

Phil Evans, Martin Noble, Stuart McNicholas, Keith Wilson, Garib Murshudov, Kevin Cowtan, Raj Pannu, Pavol Skubak, Frank von Delft, Eleanor Dodson, Fei Long, Harry Powell

Eugene Krisseneel, Charles Ballard, Martyn Winn (First set of items only)

Absent: Dave Rice.

1 Funding status (CB)

There is enough money to support 2 posts. Charles has already factored the likelihood of needing to support Stuart after 2011.

2 Prioritisation for core activities (EK)

There was a rehash of many of the issues discussed above.

The core team is far too heavily burdened by the download questions, and it is urgent to find a solution, both to simplify the procedure for users, and to free up the core team for more interesting activities.

Eugene was interested in a Virtual Machine solution which would allow inexperienced users to access the programs without downloading them, but the Exec felt there would be many exceptional cases.

3 Proposal for extra core post

Eugene presented a proposal. It was rather vague, so although the Exec was sympathetic, he will be asked to rewrite it with clearer aims. The grant had envisaged one core post (Peter Briggs) being used to support GUI development. There is also the suggestion of a Diamond/CCP4 jointly funded post. One area for cooperation would be new data processing software. Maybe Andrew Leslie and Gwyndaf Evans should make a joint proposal? Another area would be in developing EDNA, but discussion on this was deferred till after a decision is made re EDNA. Frank felt CCP4 might have other urgencies, in particular addressing the underlying chemistry used by structure, which might require further support for the Ligand initiatives.

4 Progress against Grant deliverables (MN)

4.1 Model building (KC)

4.2 GUI and database (MN)

4.3 MOSFLM (PRE)

4.4 Core (EK)

Good progress against deliverables. One issue was: who is responsible – Jim Naismith or Martin Noble, and when is a report required? Martin will get in touch with Jim and find out what is needed.

5 CCP4 challenges

5.1 The competition

Serious but also provides a challenge.

5.2 GUI and database. EDNA & Pipelines

See procedures outlined above, and Martin's summary below. It is important to keep Alun and Diamond in the loop.

5.3 Installation

Must be solved but not clear yet how. Eugene suggests a software freeze after the next release to allow core team to investigate a better method.

5.4 Program output

Tables and loggraphs – Liz and Phil will report – When?

5.5 Coordination of effort

Was there a plan?

5.6 Ligands

A wide ranging discussion, with no firm conclusion.

Appendix:

Martin's Email.

Thanks for attending the CCP4 developers meeting: we know that discussing data models is less fun than writing code.

It would probably be helpful to summarise decisions about how CCP4 developers implement and will deliver workflow elements.

We are committed to developing a shared data model with Diamond/EDNA

- Garib and Fei will draft preliminary UML/XSD with reference to DIMPLE
- This will be checked into the EDNA SVN, for comment by Graham, Liz, Raj et al

We are committed to delivering CCP4 functionality to EDNA pipelines: early deliverables (1-2 months) will be

- Ronan will provide DIMPLE and MrBUMP wrapped in EDNA
- Fei will provide EDNA-factored BALBES

For all future pipelines

- CCP4 will provide EDNA-wrapped forms of the pipeline

Fei, Ronan, and Graham all provided positive feedback about EDNA as an environment to work: by the end of the meeting, there was consensus that the challenges of EDNA that were apparent in the workshop might be superable. As such, the working model is that CCP4 will adopt, and encourage adoption of EDNA as the framework with which to construct workflows.

A final decision on whether to do this will be made by end May: we need to establish that improvements, actual or planned, to EDNA and its documentation have addressed concerns about useability, convenience, and barrier to entry. These concerns are made

more immediate by the confirmation that industrial users (our main sponsors) want CCP4 function to be provided in wrappers that they can be easily learned and readily deployed in their own workflows.

The decision will be made by the exec committee based on feedback on a code-analysis of DIMPLE and EDNA-BALBES. We'd like to invite written reports from Fei and Ronan (best positioned to report on the pros and cons of EDNA to an adopter). It would also be helpful if Liz (who will have to connect pipelines to a GUI) and Eugene (who will lead the team tasked with maintaining and implementing substantial code) could evaluate the DIMPLE code and discuss with Graham and the EDNA team any ways in which it might be further improved before providing further reports.

Reservations notwithstanding, the meeting lifted my gloom about whether there was a good way forward. I am really grateful for the give and take there has been by all parties in starting to agree a way we can all work effectively together.