

CCP4 WG2 Meeting - 3rd July 2013

Present: Andy Purkiss (CRUK), Alun Ashton (DLS), Ralf Flaig (DLS), Iwo Tews (Southampton), Liz Potterton (York), Eugene Krissnel (CCP4), Michel Isupov (Exeter), Stuart McNicholas (York), Marcin Wojdyr (CCP4), Arwen Pearson (Leeds), Chris Wood (CCPEM), Charles Ballard (CCP4), Ville Uski (CCP4), Ronan Keegan (CCP4), Carol Malpass (STFC)

Apologies: Frank von Delft, Nick Keep, Lindsay Sawyer, Johan Turkenburg, Phil Evans

Birkbeck College at 11:30am.

Room G15 in the main building.

Tea and coffee available from 11.00am.

Agenda

11:30am Start

1. Update from Core team (Eugene)

** CCP4 exec have decided to support Raj Pannu's grant application with in kind funding.*

One new post between DLS and CCP4 to promote collaboration and push forwards Dimple and other pipelines. This is in progress.

** APS workshop just completed (6th Workshop at APS) was very successful. They want to expand the course to include other beam lines (currently associated with GMCA-CAT). Next year more will be involved, but only for lectures, practical classes will remain limited.*

** Final stages of prep for 6.4.0 release. Major component will be integrated updater. Lots of people had updater installed, but never managed to update. Refmac, and others will have upgrades. Also integrated COOT for unix in the release. Coot is now integrated for all three major platforms. Anticipate the release will be in July. Still need to tidy Crank and Mg.*

** Upcoming workshops at Oulu in September (Andrey going). Okinawa (November). Posters at ECM + 1 talk and a seminar at the computational crystallography course. No stand - too expensive - will use posters instead.*

** SW proceedings. 2012 in press July issue. 2013 6 accepted, 2 on final revision, 3 back with the authors. 3 still awaiting referee comments.*

2. Study Weekend 2014 (Ivo)

New organiser team - Ivo Tews and Jon Cooper. Ivo gave a presentation about his plans for the SW. These met with general approval. Suggestions for further speakers to Ivo by the end of July.

3. GUI2 demo (Liz Potterton)

Liz gave a demonstration of ccp4i2. She showed a number of programmes within the gui. Some nice interfacing to coot and mg. Can also upload xia2 data. Showed how to navigate the GUI, how to rename objects and jobs.

4. GUI2 General discussion and release prospects (Liz/Eugene)

** MiniMTZ files. Attempts to remove user confusion by splitting out different aspects of the mtz file by treating columns very differently. Charles asked about provenance and consistency checking to ensure phases are associated with the correct structure factors etc. Are still some problems with programs not being willing to accept all forms of experimental data etc. Ccp4i2 does the conversions internally to support the different programmes.*

** Dependencies - ccp4mg, CCP4, Coot, hklview, pimple (new loggraph). When gui2 is released then all these will be included in the bundle. As long as people are using the updater (bundled version of ccp4) then gui2 should play nicely with 6.4.0 onwards.*

**** What's missing?**

Experimental phasing structure determination

Building/importing ligands

Documentation fuller reports

Mosflm - should be able to call this, and get info pushed back into the database.

**** Core features planned**

Capture workflow and repeat (branching jobs)

Tree view of project and querying of the project

Review/comparison of MR models/"final models" etc.

**** Platform issues**

Windows build still not great - don't play with that yet.

Unix/mac users please play and send feedback to Liz. Liz will release further test versions to wg2 with instructions as to what she'd like people to try. Please do so and feedback.

**** Please feedback to Liz about which programmes/pipelines you'd like to see in the gui2.**

Liz also asks for small structures for demo purposes - soluble by MR ideally with a ligand and with some xia2 output. Charles suggests the BESSY tutorial data.

**** Requests from wg2**

Provide output from a molprobit or other validation run straight on the end of the refmac run and link from this into Coot. Quicker identification of problem areas of the structures.

Easier access to log file for each job?

Access to command scripts and option to edit them?

5. AOB

Next meeting - last week of January 2014, Leeds.

To include:

* Gui2 short demo (Liz)

* Demo imosflm multiple lattice stuff. (ARP to approach Harry).

3:30pm end.