

Meeting title	CCP4 Working Group 2 meeting (chaired by Arnaud Basle, University of Newcastle)		
Date	Wednesday 21st of June 2023	Time	11.00 – 13.00
Location	Virtual only	Zoom	yes
Circulation	ccp4wg2@stfc.ac.uk		
Attending online	Jon Agirre, Arnaud Basle, Clemens Vornrhein, Karen McIntyre, Charles Ballard, Helen Ginn, Alan Roseman, Roberto Steiner, Pietro Roversi, Luiso Fuentes-Montero, Ville Uski, Isscu, zrid30b, Nicholas Pearce, Eleanor Dodson, Christoph Mueller Dieckmann, Anna Warren, Eugene Krissinel, Petr Kolenko, Paul Bond, Robbie Joosten, Dave Briggs, Stuart McNicholas, Ed Lowe, Airlie McCoy, Paul Emsley, Andy Purkiss, Briony Yorke, Svetlana Antonyuk, Keitaro Yamashita, Rob Nicholls, Dan Rigden, Gustavo Lima, Maria Fando, Ralf Flaig, Ronan Keegan, Marcin Wojdyr, Hanna Kwon, Mark Roe, Ben Bax, Peter Moody, Martin Mâly, Ralf Flaig, Ivan Campeotto		
Apologies from	Mike Hough, Ivo Tews, Johan Turkenburg, Ed Lowe, David Waterman		

10.00 Welcome

10.05 Chair's update

Last meeting's minutes: these were circulated and amended shortly after the last meeting. We hear no complaints, so the minutes are

10.15 CCP4 updates

Charles: New release towards the end of this year, updated Python (3.9) and new compiler version (this will likely fix issues affecting certain software such as Tortoise and Iris). Adding Rope likely (Helen to comment). Coot 1.0 being rewritten for GTK 4.

Paul Emsley: We might have something in November. Would be good for CCP4 to provide binaries for friendly critics to comment on developments.

Charles: Andrey working on localisations/Windows towards the next release. Test bundles will be available from this CCP4 Download page:

 <http://devtools.fg.oisin.rc-harwell.ac.uk/downloads>

Note that this is NOT ccp4.ac.uk but the server that hosts the builds

The idea will be to put GTK 4 Coot builds in there for people to test.

DUI 2 to go into the next release?

Luiso: would like to do at least a 'silent release' (we release it but don't tell anybody about it, *shhh*).

10.35 CCP4 Study Weekend 2023 (Christoph Mueller)

Lots of papers confirmed (well done!), with just a couple going into September – no worries about this, every year there are a few papers submitted late. This problem was mitigated with the introduction of virtual issues and immediate electronic publication.

10.55 **CCP4 Study Weekend 2024 (Clemens Vonnrhein)**

Karen: other venues (*e.g.* Leeds) were evaluated, but it looks likely that we will repeat at EMCC Nottingham. Some people suggest that the improved spaces at the EMCC were very comfortable.

Clemens: title still under discussion. Current idea: "Decision making in MX: how to be a productive structural biologist". Flow to match a 'from crystal to structure' kind of meeting, but with a focus on decision making.

Heavy use of automation to be discussed in Day 1 late afternoon. Lots of SARS-CoV-2 research to be featured.

Panel discussion to be kept: Has AI changed the direction of structural biology and MX?

Ivo: good to keep the panel, also forces a few PIs to attend.

Clemens: idea will be to prepare pre-questions that people can answer, engage with virtual participants too.

Ed Lowe agrees.

Dave Briggs: I have attended meetings at the Royal Institution where live votes have been done.

Arnaud: we could make the questions part of the registration process, although admittedly many people do get registered very late. But anyway most will be ready before the holidays, so still time for the panel to think about them.

Clemens: test run on WG2 mailing list.

Arnaud: panellists, do you want suggestions from WG2?

Clemens shows the list of proposed speakers (*omitted from minutes*).

Dave Briggs: Are we considering discussion of autobuilding pipelines as well? Modelcraft?

Discussion on the panel, issue with it running parallel to the Diamond User meeting.

12.15 **Northern meeting (Ivan Campeotto)**

26 & 27 October, Jubilee hotel in Nottingham.

May need to charge students.

Flyer is ready, just waiting for sponsors.

Call for lunchtime bytes.

Arnaud: that will incur a cost due to room usage.

12.55 **Any other business**