CCP-EM Working Group 1

Harwell, Tuesday 25th April 2017

Minutes

Summary of Actions

Please alert Martyn Winn or Tom Burnley to anyone who should be included in WG1, and is not yet.	All
Post minutes of CCP Steering Panel meeting, December 2016	Martyn
Plan a meeting on tomography in CCP-EM	Martyn et al.

Present: Radu Aricescu, Alun Ashton, Morgen Beeby, David Bhella, Doryen Bubeck, Per Bullough, Liz Carpenter, Megan Dowie, Juan Fontana, Kay Grunewald, Pradeep Luther, Carolyn Moores, Edward Morris, Stephen Muench, Lori Passmore, Simon Phillips, Alan Roseman, Peter Rosenthal, Helen Saibil, Christiane Schaffitzel, Corinne Smith, Laura Spagnolo, Dave Stuart, Ian Tickle, Maya Topf, Martyn Winn, Giulia Zanetti, Peijun Zhang.

1. Overview of CCP-EM activities

Colin Palmer joined the core team in August 2016. Colin did his PhD at the MRC LMB on a novel specimen holder for electron cryo-tomography, followed by two years as a software engineer at Diamond in the Data Acquisition software team.

The first CCP-EM Developers Workshop was held at Cosener's House on 3 – 5 Oct. 2016 and was attended by 23 scientific software developers. This included those in the CCP-EM community, as well as EM-curious developers from CCP4. Topics discussed included overlaps between several python libraries that have been developed, testing frameworks, image compression, and map / model validation.

A CCP-EM associated BBSRC grant, "Automated de novo building of protein models into electron microscopy maps" Cowtan (York) and Winn (CCP-EM), started in February 2017.

A beta-release of the CCP-EM software suite has been made, mainly covering model fitting and building. A small stand-alone Python library for handling MRC format files has also been written by Colin, and released on Github https://github.com/ccpem/mrcfile.

2. Planned training activities

Recent workshops:

• A one day RELION workshop led by its developer Sjors Scheres and hosted by CCP-EM and the Astbury Biostructure Laboratory (University of Leeds, UK) on 19th September 2016. The workshop included a tour of the new cryoEM facility there.

- Biochemical Society Training Day: Advanced Data Collection for High Resolution cryoEM: How to make the most of your National Facility Visit. This was organised with eBIC and CCP-EM and held at Diamond Light Source on 6 September 2016. The course was aimed at users and potential users of eBIC (electron Bio-Imaging Centre) at Diamond, and covered all stages from sample preparation to structure solution.

- Icknield Workshop on Model Building and Refinement for High Resolution EM Maps, held at Harwell 5-7th April 2017.

Planned workshops:

"Instruct Workshop on cryoEM best practices", 9th-10th May, Harwell. Workshops are open to facility managers, scientists in the field and database specialists, from both academia and industry (max. 30 participants), and this first one will concentrate on data management and analysis. Martyn will talk on CCP-EM.

Joint workshop with CCPBioSim at Leeds, July 2017.

"Methods and applications in the frontier between MX and CryoEM" organised by Isobel Uson and Garib Murshudov, Sept 2017. Tom will speak on CCP-EM.

3. Options for Spring Symposium 2018

The first three Spring Symposia have been held on the Harwell campus. Although these seem to have been successful, there are two limitations: Firstly, the lecture theatre has a maximum capacity of 200. Secondly, accommodation in the area is limited, and delegates have to be split over at least two hotels. Other venues provide larger lecture theatres, and on-site accommodation, but are more expensive. At Harwell, the lecture theatre and side meeting rooms are free, and we pay for catering, AV assistance, speakers costs and bus transport. This year, we have charged a modest registration fee (£150 / £75) so that the net cost to CCP-EM is around £3k.

The pros and cons of moving the Spring Symposium off-site were discussed. Points raised included: keep student costs down, look for sponsorship, can we used an overflow room at the Harwell site, would we consider hosting the meeting abroad.

There was support for both keeping it a small meeting on the Harwell campus, and also for trying to grow the meeting as a national event. There was probably a slight preference from WG1 for the latter.

It was suggested to talk to learned societies (Biochemical Society, RMS), who may be able to give travel bursaries for members.

4. Spring Symposium Proceedings

We were requested at the last meeting to consider other journals for the Proceedings of the Spring Symposium. We approached JSB, who informed us that they would charge USD 2600 per article for open access, and would not give us a discount.

Acta Cryst D expect us to publish articles as Open Access, but will give us a 50% discount on the usual fee of USD 1200. However, they will waive the fees for the first edition, i.e. the proceedings of

the 2016 meeting. From this year onwards, we will need to pay OA fees. The CCP-EM grant cannot cover all of this, so we will rely on the majority of authors accessing institutional funds.

The proceedings of the 2016 meeting are planned for the June edition, and the first 5 articles are now available online (see http://journals.iucr.org/d/issues/2017/06/00/).

5. Interactions with eBIC

Laura Spagnolo is eBIC representative on the Diamond user committee. They have two meetings per year, with the first meeting in March. Discussion topics included vending machines, 3 month turnover of applications, automation pipelines.

David Bhella, Lucy Collinson, Helen Saibil are on the STFC soft matter committee. They would welcome comments for STFC on funding, facility support.

Tom and Colin hotdesk for half a day per week in the new eBIC building, and there is also a monthly IT coordination meeting involving staff from eBIC, CCP-EM and Diamond computing.

Tom and Colin have been involved with installation of software (available via "module load"). They have also benchmarked Relion 1.4 / 2.0, and trialled an installation of cryoSPARC.

6. Interactions with EMDB

Ardan for EMDB has deposited several tools in the CCP-EM code repository https://ccpforge.cse.rl.ac.uk/gf/project/ccpem/scmsvn including an XML translator between versions of the EMDB data model, and software for the proposed Segmentation File Format.

Peter Rosenthal summarised an application to the Wellcome Trust (now funded) looking at validation tools and services for cryoEM. This will cover map vs image and model vs map validation. The grant is for tool development, rather than pure research.

There was a discussion on capturing metadata about the experiment, which led on to a discussion about using quick assessments of data to feedback to data collection. Whether users can act on this depends on how long screening takes. There is a potential impact on eBIC staff if it leads to extra screening.

7. Report from CCP Steering Panel

Peter attended the Dec 2016 meeting of the CCP Steering Panel on behalf of CCP-EM. The purpose of the panel is to encourage collaboration between the different CCPs. CCP-EM should consider links with CCPI, CCP-SAS and CCP-PetMR. Martyn to post minutes on the CCP-EM website.

8. AOB

Kay suggested a meeting to make plans for CCP-EM in the area of tomography. There should be more on subtomogram averaging.