CCP-EM Working Group 1
Nottingham, Tuesday 30th April 2019
18:00 – 19:00
Minutes

Present: Martyn Winn, Tom Burnley, Colin Palmer, Sjors Scheres, TJ Ragan, Doryen Bubeck, Corinne Smith, John Briggs, Martin Walsh, Randy Read, Anne McGavigan, Giulia Zanetti, Pamela Williams, Andy Purkiss, Peter Rosenthal, Neil Ranson, Maya Topf, Alan Roseman, Danielle Paul, Carolyn Moores, Edward Morris, David Lawson, Gerard Kleywegt, Gerard Bricogne, *et al.*

Apologies: Helen Saibil

CCP-EM Software Suite highlights

There was a discussion around hardware requirements and computational infrastructure. It is hard for CCP-EM to provide a one-page answer for "what should people buy" since it depends on many factors. Erik Lindahl provided a useful blog on GPU platforms for Relion, but even that is no longer up-to-date. A more practical approach would be for labs to provide descriptions of their own computational setups, particularly if setting up a new facility, which CCP-EM can disseminate as exemplars for others. CCP-EM could provide a template for this.

Does CCP-EM plan an update mechanism for the suite, such as CCP4 have? This potentially could take some time to get working robustly, and we have prioritised others developments, but in the long term we'd like to do this.

Does CCP-EM plan to support cloud computing, e.g. by providing images are containerised applications? In principle yes. There has been an exploratory project with the STFC Scientific Computing Dept but this is not suitable for production.

Does CCP-EM plan to distributing libraries for machine learning e.g. Tensorflow? We have recently hired a machine learning specialist, so we will need to address portability of machine learning code and models at some point.

Workshops

The current set of teaching workshops was summarised. Should we have a set curriculum that we cycle through in 2-3 years? All workshops are over-subscribed, so perhaps we should focus on giving more of these rather than expanding into other areas? The main limit is the free time of the core team. We are happy to support (via finance, tutorials or admin help) workshops organised by others.

A tomography workshop given by experts would be a good use of money and time. After the meeting, a workshop on SerialEM was also suggested. It is hard to get David Mastronarde over. One option is to use Nexperion who offer training for SerialEM and IMOD.

Spring Symposium 2020

Nottingham Jubilee campus is already booked again for next year. Feedback for this year's event has been good, except for the catering. In particular, the mixer event did not allow much mixing, and the conference dinner was not special.

Many people who attended the eBIC User Meeting on the first day did so by accident, having turned up early for the main meeting.

Everyone appreciates the time for informal discussions and networking. Some wanted more free time for this, while others felt that there was enough. There was some support for Lunchtime Bytes, where software developers can demo the latest features and/or hold a clinic for problems. These are run at the CCP4 Study Weekend and are popular, though do put more pressure on the schedule.

Scientific organisers are required for next year. John Briggs commented that the organisation is easy, thanks to the support of the core team!

Commercial income

Following the CCP4 model, the CCP-EM suite is licensed free to non-profit organisations and for a fee to for-profit organisations. To-date, we have 11 licencees giving a potential income stream of about £50k. This is not yet enough to fund major software development projects, but can support some CCP-EM activities.

The greatest support was for co-funding PhD studentships at collaborating universities. At least part of the PhD should include method or software development of interest to the CCP-EM community, ideally something that can be included in the software suite.

Alternative ideas included funding short (few month) development tasks e.g. making use of RSE effort; subsidising more workshops or community meetings; student bursaries for conferences; and funding placements e.g. at Diamond.

Wellcome Trust validation grant

There was a brief overview from Peter Rosenthal. The grant is contributing to a community-wide effort to agree on tools and metrics, which can then become part of deposition and be adopted by journals.

There is a question of how the wwPDB can find an EM representative for their board. They currently approach the IUCr for crystallographers, but there is no equivalent organisation for cryoEM. One suggestion was to vote on it at the GRC, although this is not ideal as attendance at the GRC may be skewed.

Grant renewal

The current grant ends in February 2021. Assuming we apply to MRC again, we should aim for the January 2020 deadline for submission.

There was a discussion on possible themes. The case can include infrastructure developments, though it also needs to be seen as science-driven and leading edge.

One idea is to have an integrated pipeline to go from raw data to deposition. Part of this is being built already, but it would be good to make it better integrated with proper workflows instead of single GUIs. It would be timely to include a machine learning component. One aim should be to provide rapid feedback to the data collection at the microscope.

Users would appreciate support in moving data between packages. We have been cautious in promising to support all cryoEM software, as this would be a major time sink for the core team and would be hard to keep up-to-date. Nevertheless, some support for a subset of programs should be possible. A workflow engine could help here.

Should we consider other scientific directions? Electron diffraction is being supported by CCP4, as there strong overlap with X-ray diffraction structure solution. Electron tomography is more relevant for us, and will be important in the 2021-2026 timeframe of the next grant. John Briggs felt that this might happen organically, as the line between single particle analysis and sub-tomograph averaging gets blurred.

The grant currently funds Tom and Colin (plus a small percentage of Martyn and some admin support), who cover all activities including algorithm and software development, training, Spring Symposium and some local support for eBIC. If we can demonstrate community demand, then it would be useful to expand this team.

AOB

None.