

CCP-EM Working Group 1

Keele, Wednesday 11th April 2018

Minutes

Summary of Actions

Please alert Martyn Winn or Tom Burnley to anyone who should be included in WG1, and is not yet.	All
Select scientific organisers for 2019 Spring Symposium	Peter + core team

Present: Martyn Winn, Danielle Paul, Raffaella Carzaniga, Alun Ashton, Carolyn Moores, Edward Morris, Alan Roseman, Peter Rosenthal, Helen Saibil, Corinne Smith, Sasha Bakker, Giulia Zanetti, Peijun Zhang, Neil Ranson, David Lawson, John Schwabe, TJ Ragan, Martin Walsh, Dan Clare.

Apologies: Juan Fontana, Sjors Scheres, Maya Topf

Martyn's update on CCP-EM activities is attached as a separate document.

1. CCP-EM software suite

Version 1.0 has just been released. This provides the basic framework of the suite and initial functionality around model building and refinement. There was a discussion on future directions.

High on the list is inclusion of Relion. Sjors is happy in principle but there is an open question on how we can provide some added value to the existing (very good) Relion package. Seamless integration with model building would be one major plus, especially where there are multiple maps from classification or focussed refinement. There was a request for CCP-EM to distribute the most recent version of Relion along with all major stable releases (Scipion does something similar).

Imminent additions to the CCP-EM suite include LocScale, emClarity and SuRVoS. The latter will help us start to provide support for tomography. There was a request for us to look into including NovaCTF.

Version 1.0 has been released with not-for-profit and commercial licences. There are plans for the latter to have a modest fee of £5k. The aim is to generate an income stream for the project, rather than full commercialisation. The meeting was supportive of this approach.

2. Spring Symposium

This year is the 4th edition of the Spring Symposium, and the first time we have moved off the Harwell Campus. Attendance has been roughly 100, 150, 190, 190 over the 4 years. Thus attendance has not increased this year, which is possibly due to the timing in the Easter holidays. We still expect an increase in attendance for next year, and Nottingham Jubilee Campus has been booked for the 29th April to 1st May 2019.

The meeting discussed three proposed changes. Firstly, there will be an eBIC user meeting on the first day before the main CCP-EM meeting. This mirrors the successful MX user meeting before the CCP4 Study Weekend. This was agreed to be a good idea. Secondly, we will again invite people to bring posters, with a poster session perhaps on the first evening after the eBIC user meeting. This could be supported by pizza and beer. Thirdly, we will select 2 or 3 scientific organisers from the community, rather than the scientific programme being organised by the core team. The core team would continue to organise the event itself, with the scientific organisers responsible for suggesting a programme and liaising with speakers. The suggested programme should be shared with this group (i.e. Working Group 1) before inviting speakers, for approval or to request additional suggestions. The meeting agreed that the Spring Symposium should continue to cover all of cryoEM, rather than focussing on a particular topic.

3. Planned training activities

The demand for training courses is still greater than CCP-EM can deliver. This is partly to do with funding, but mainly the time taken to organise a course, which takes away time for other activities such as software development. Regional centres have the same issues. Joint workshops between CCP-EM and a regional centre would make it easier for all. As a recent example, there is a GW4/CCP-EM Relion workshop at Bristol, May 2018, which is modelled on a similar workshop in Leeds in 2016. At Leeds, the Sjors-led day was followed by a second day in which the tutorial was repeated to local users.

4. Interactions with eBIC

Tom and Colin hotdesk in I14 building on Weds afternoons. Those who are at eBIC are encouraged to visit them. Katie Cunnea has organised a meeting on the second day of the Spring Symposium to investigate ways for facility managers to interact more, and share knowledge.

5. Interactions with EMDB

The meeting agreed that CCP-EM should work with EMDB on validation and deposition. The aim would be to reduce the activation barrier for preparing data and metadata for deposition. We can help to encourage people to deposit all relevant maps, e.g. for focussed refinement.

6. Other collaborations

Several CCP-EM partners have formed a consortium to look at validation, which has been funded by a WT Technology Development Grant. The grant has just started, and progress will be reported to future meetings.

STFC core support for CCPi and CCP-PetMR are now part of Martyn's group at STFC. This raises the possibility of cross-CCP projects. There was only a brief discussion on this, but the initial reaction was that there is little overlap, due to the distinct samples and scientific aims.