CCP-EM Working Group 1
Friday 6th May 2022
11:00 – 12:30
Minutes

Attendees:

Martyn Winn, Neil Ranson, Per Bullough, Tom Burnley, Charlotte Scarff, Ciaran McFarlane, Colin Palmer, Gerard Kleywegt, Nobu Morone, Pradeep Luther, Corinne Smith, Randy Read, Yuriy Chaban, Alistair Siebert, Agnel Joseph, Maya Topf, Matt Iadanza, Giulia Zanetti, Helen Saibil, Henryk Korza, Jerome Gouge, Juan Fontana, Marcus Wilson, Mark Basham, Natasha Lukoyanova, Panchali Goswami, Sjors Scheres, Andy Purkiss, Carolyn Moores, Peijun Zhang, Robert Deller, Roberto Steiner, Peter Rosenthal, Chun-wa Chung, Kyle Morris.

Introduction

Martyn summarised the current management group of CCP-EM. Besides the original 10 investigators on the MRC grant, Giulia Zanetti has joined as a new CoI following Maya's move to Hamburg. In addition, Pamela Williams has been co-opted as an Industrial Representative. Her remit is to communicate industry priorities to CCP-EM management, and help disseminate CCP-EM activities to the industrial community. Members of the community are encouraged to approach anyone from the management group with concerns or questions.

Future plans for the CCP-EM software suite

Tom Burnley summarised the plans for the CCP-EM software suite, in particular the recent release of v1.6 and plans for the new Pipeliner.

Neil asked about plans for ensembles of structures, in particular in the context of the deposition tool. CCP-EM developers met with Ardan and his team in September 2021, and we'll reach out again now that the deposition tool is starting to take shape. Matt stated that it would be easy to update the schema used by the deposition tool, to keep it in line with PDB/EMDB/EMPIAR requirements. The community also has the possibility of influencing what is held by the archives via EBI meetings, or via CCP-EM. Maya suggested that we should begin to plan for more small molecules located in cryoEM structures. Gerard reminded us that wwPDB is a supertanker, and we should engage as early as possible.

Neil reported problems with Coot v1 on Macs. These are known, and Charles Ballard (CCP4) is working on it. Colin asked whether CCP-EM should continue to distribute its own build of Coot. The original reason was to include recent changes relevant to cryoEM, but now these are available in the CCP4 version. However, there was support for CCP-EM keeping its own version, for those that rely less on CCP4.

Tomography pipelines

CCP-EM hosted a workshop for developers at the end of March on the use of the Pipeliner framework for tomography. Sjors commented that the workshop was great, and he is working on improving the import of tomography data into Relion for subtomogram averaging. This would reduce the amount of processing needing to be implemented in the pipelines. Others stressed that it would always be necessary for some projects to step outside of Relion, and the Pipeliner should be able to support this. Particle picking from tomograms was highlighted as being very project-dependent.

The plugin architecture of the Pipeliner was designed to allow others an easy way to incorporate 3rd party tools. CCP-EM core staff can help with this, but don't want to support all tools and workflows. Nevertheless, the CCP-EM suite should eventually support a few alternative pipelines using different software.

Training

Martyn summarised a list of events with CCP-EM involvement. Maya asked for the Hamburg EMBO course on Practical integrative structural biology to be added. Martyn also summarised a discussion between CCP-EM and the WT-MRC training consortium on coordinating efforts. While the latter have a broader remit (i.e starting from sample preparation), CCP-EM can help with training on processing software and on general admin.

STFC are hosting an "EMshare" sharepoint site for use by the WT-MRC training consortium, CCP-EM and others in the community. It is currently being populated with a first set of resources and tested, and will be formally announced later. There is a brief authentication process to obtain access to the site.

Kyle said that they had agreed to not store any data on EMShare, but rather they would link out to e.g. EMPIAR. Tutorial data may be trimmed compared to the original dataset in EMPIAR, so the question is whether the tutorial data can be added to the existing entry, or whether a new entry should be created. Gerard asked people to get in contact to discuss the best way.

Sjors was asked about a Relion 4 tutorial. He is waiting for the software to be completely stable. In particular, the import of tomograms needs to be made smoother (see above). CCP-EM staff could do one based on the Pipeliner framework when that is ready. Kyle commented that they have a Relion 4 tutorial starting from the output of eBIC automated processing. Peijun has just published a protocol based on a trimmed dataset that could also be made into a tutorial.

Corinne asked for links to resources for basic compute training. The CCP-EM website has a Linux cheat sheet, created for students new to command line processing. Mark mentioned that the Software Sustainability Institute has resources on software carpentry including basic introductions (https://www.software.ac.uk/resources/training-resources).

Finances

Martyn summarised the income sources for CCP-EM, which include the main MRC grant, income from commercial licences, and additional grants associated with CCP-EM. The main expenditure concerns software developers, training and events.

We are able to fund small software development projects, and have previously supported projects at York and Birkbeck. We do not run formal calls, but the possibility for funded collaboration is advertised on the front page of the CCP-EM web site. Proposals are considered by the CCP-EM management group. Sjors stressed the need to continue support for the Pipeliner, and to have effort available to oversee plugin development by 3rd parties.

Spring Symposium

We are now looking for scientific organisers for 2023. We look to balance gender, geography and science. Giulia suggested someone from the southwest GW4 consortium. Other suggestions can be emailed to Martyn or anyone else in the core team.

Regarding the programme, there was general support for plenty of breaks to allow for informal discussion. There was some debate about the poster session, which was felt to be in a remote location coupled with no dedicated time. At least one of the coffee breaks could be held at the posters. There was some interest in software demonstrations which could be held alongside the posters. We need to balance additional activities with free time for socialising.

Yuriy asked about a roundtable session to discuss specific issues (e.g. map deposition or time resolved studies). eBIC held a roundtable at the end of the first day.

The East Midlands Conference Centre has already been booked for next year (25-27th April), in order to secure the preferred dates. It will almost certainly be hybrid again. This is good for accessibility, but does impact the finances. We need a minimum of 150 on-site attendees to make the large venue viable. This year, we had 150 registered for in-person, of which 144 turned up. We had 914 registered for virtual attendance, though in fact we had 1140 unique views on Zoom. Numbers were probably impacted by continued uncertainty around the pandemic, and hopefully we can increase that next year. There was a feeling that there were fewer PIs and senior developers at the meeting, which could be disappointing for students.

Maya asked whether we should charge a small fee for online attendance, and perhaps encourage some to come in person. Charlie suggested we look for organisers for 2024 as well, to give a longer lead time for organisation. It was also suggested that we could have a poster prize.

AOB

There was no other business.