

MS04-P01 | CCP-EM: THE COLLABORATIVE COMPUTATIONAL PROJECT FOR ELECTRON CRYO-MICROSCOPY

Winn, Martyn (STFC, Didcot, GBR); Burnley, Tom (STFC, Didcot, GBR); Palmer, Colin (STFC, Didcot, GBR); Joseph, Agnel (STFC, Didcot, GBR); Mirecka, Jola (STFC, Didcot, GBR)

The Collaborative Computational Project for Electron cryo-Microscopy is a community project to support computation in cryoEM. It is modelled closely on the long-running CCP4 project for MX, but is separately managed and with a remit to include all cryoEM modalities from high resolution single particle analysis through to tomography. I will present an overview of CCP-EM activities, together with two specific projects in the key areas of validation and machine learning.

The CCP-EM software suite is currently focussed on single particle analysis. It combines pre-processing and reconstruction in Relion with building of atomic models. Several workflows are possible, depending on the resolution of the cryoEM map and the availability of atomic models. Some crystallographic programs are included, which have been adapted to take into account different map distributions and lower resolution.

CCP-EM is a partner in a validation consortium which is developing tools for validating cryoEM reconstructions and fitted atomic models. Together with the EMDB, CCP-EM is responsible for disseminating these tools to the cryoEM community. We have developed a set of tools for the CCP-EM software suite with the aim of catching problems early, and anticipating future deposition requirements.

As an experimental technique generating large and numerous datasets, cryoEM is ripe for the application of machine learning. We are developing machine learning models for recognising features in cryoEM maps, at a range of lengthscales from components of complexes down to individual side chains. We are investigating the dependence of these models on data quality and resolution.