



CCP-EM

Report to WG1 - April 2018

Martyn Winn

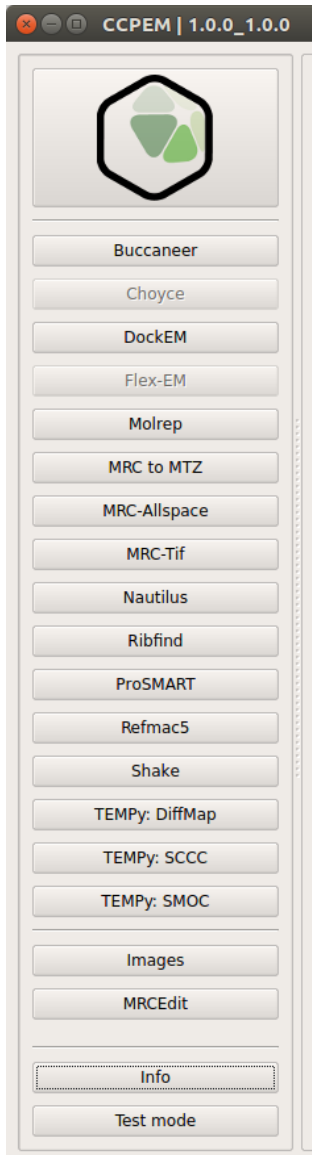
1. Software Suite

Version 1.0 released

- Focussed on model fitting, building, refinement, validation
- Integration with molecular graphics packages (Chimera, Coot, CCP4mg)
- Some utilities for images
- Command line

Current USP but more to come

Developers: Tom, Colin, Alan Roseman, Maya Topf, Agnel Praveen Joseph, CCP4 developers



Usage

- Downloads
 - no accurate statistics for beta release
- Queries to `ccpem@stfc.ac.uk`
 - approx 1 or 2 per week, from e.g. Oregon, Janelia, Case Western, Munich, Utrecht, RCaH, CICbioGUNE, ICR, MPI Frankfurt, etc (from random selection of emails)
- Citations
 - TMEM16A channel, *Nature* Dec 17, "Reciprocal space refinement was performed with Refmac incorporated in CCP-EM."
 - initiation factor eIF2 α , *Science* Mar 2018, "REFMAC in CCP-EM was used to further refine the model and automatically generate the map vs. model FSC curves"
- Used in Icknield workshops, Instruct courses

Licensing

- CCP-EM has umbrella licence, included packages can be licenced differently (often Open Source)
- Academic / non-profit and commercial / for-profit versions
- Always free-of-cost to academic / non-profit
- Modest charge to commercial / for-profit
- Follows the CCP4 model. Aim is extra support for activities, not to make a profit.
- Discussed with: MRC, STFC, grant holders, pharma companies, CCP-EM developers, CCP4 developers and executive committee

Plans in progress

- Relion (Sjors)
 - pipelines being developed
- LocScale (Arjen Jakobi)
 - local sharpening, in release but hidden
- ProSHADE (Michal Tykac)
 - detection of local map and model symmetry
- emClarity (Ben Himes)
 - sub-tomogram averaging, agreed inclusion, Matlab and GPU dependencies
- SuRVoS (Mark Basham)
 - tomogram segmentation, agreed inclusion

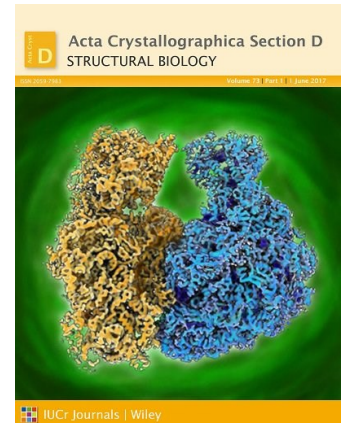
Discussion points ...

- Direction of software suite
 - expand beyond model building
 - usual caveats: don't reinvent wheels, finite developer time
- Licensing
- Other models of computational help
 - reference installation cf. SBGrid
 - web services

2. Training courses

- Icknield workshop on model building, Harwell, 5th - 7th Apr 2017
- Combining EM and MD Workshop, Leeds, 13-14th July 2017
- EMBO, Birkbeck, 5 – 15 Sept 2017 (sponsor £3000, Tom speaking, Colin helping)
- CeBEM/CCP4 workshop, Uruguay, Nov 13 - 23, 2017 (Colin talk)
- Dynamo 2, Harwell, Nov 28 – 29th 2017
- Instruct / Icknield workshop on model building, Harwell, 1st - 4th May 2018
- GW4 / CCP-EM course on Relion 2.1, Bristol, 18th May 2018

Outreach, etc



2016 proceedings

- Spring Symposium 2017, 24-26th April 2017
 - proceedings due June 2018
- Instruct Best Practices, eBIC, 9-10th May 2017 (Martyn talk)
- AIC International School, Pavia, 3 to 6 September 2017 (Tom talk)
- PSI / CCP4 Workshop on electron diffraction, 18th - 22nd Sept 2017 (Colin talk)
- MX and EM methods, Barcelona, 19-21 Sept 2017 (Tom talk)
- 2nd CCP-EM developers meeting, 2-4 Oct 2017
- PSDI, 12-14th Nov 2017 (Tom)
- WT community meeting, 31st Jan (Martyn talk)
- Spring symposium 2018, 10-12th April 2018, Keele

Plans

- Spring Symposium 2019
 - Previous meetings:
 - 2015, Harwell, 100 delegates,
 - 2016, Harwell, 150 delegates,
 - 2017, Harwell, 190 delegates
 - 2018, Keele, 185 delegates
 - Nottingham already booked
 - Plans for an eBIC user meeting on Day 0
- New Wordpress website
 - easier for external editing
 - trialled by CCP4
- Video tutorials

Discussion points ...

- Format / location of Spring Symposium
- Scientific organisers
 - 2 or 3
 - CCP-EM team still provide all support

3. Interactions with eBIC

- Software on Diamond systems
 - To-date 17 packages* have been installed and kept up-to-date, available to staff and users under the module command. Some of these, for example Relion, Dynamo and CryoSPARC, have required customisation to the local compute environment.
- Running standard Relion benchmarks to check performance on Diamond CPU and GPU clusters, gaining more than a five-fold improvement in performance through optimisation of compilation and run-time options and cluster and GPU configuration
- Tom and Colin hotdesk in I14 one afternoon per week

* ctffind, motioncorr, unblur, ccpem, ctftilt, Gautomatch, cistem, Gctf, modeller, relion, coot, dynamo, motioncor2, simple, cryoSPARC, EMAN2, spider

Discussion points ...

- Pipeline development for live processing
- Joint training courses
- Interactions with other facilities

4. Interactions with EMDB

- CCP-EM package contains:
 - emdbXMLTranslator (EMDB data model)
 - emdb_sfftk (Segmentation File Format toolkit)
- Collaborations:
 - ShapeEM (started by BioMedBridges)
 - WT validation grant

Discussion points ...

- CCP-EM to contain a validation / deposition tool
 - catch validation problems early
 - capture useful metadata
 - format XML for EMDB ingestion
- Work on metadata model for structure solution
 - with eBIC
 - PDB meeting in July 2017

5. Collaborations

WT Technology Development Grant

- " Validation Tools for Cryo-EM"
- Rosenthal (PI), Winn, Roseman, Kleywegt, Patwardhan, Topf, Orlova, Murshudov
- We propose to develop and disseminate validation methodology and software tools that are now critical to support the widespread use of and investment in cryo-EM in the UK and worldwide.
- Dissemination through EMDB and CCP-EM

Other CCPs

- CCP Steering Panel meeting
 - Meets twice a year, all CCPs from all RCs
 - Minutes copied at http://www.ccpem.ac.uk/wg/working_groups.php
- CCPi and CCP-PetMR
 - CCPi: X-ray and neutron tomography for materials, links to Diamond, chair: Phil Withers (Manc)
 - CCP-PET-MR: combine MRI and PET imaging, chair: Kris Thielemans (UCL)
 - Supporting staff at STFC now in Comp Bio group

Discussion points ...

- Input to validation grant
- Overlaps with other CCPs?
 - e.g. SuRVoS used in CCPi