Research Complex at Harwell

CCP-EM

Report to WG1

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UKRI Science and Technology Facilities Council

UKRI Medical Research Council

UKRI Biotechnology and Biological Sciences Research Council

wellcome

CCP-EM grant renewal

- Submitted to Partnership Grant scheme of MRC on 8th Jan 2020, aiming for Feb 2021 start.
- Investigators: Winn, Ranson, Rosenthal, Kleywegt, Topf, Roseman, Scheres, Briggs, Zhang, Basham
- Themes: validation, sub-tomogram averaging, machine learning
- Continuation of core activities: software suite, training, community
- Expanded core team from 2 to 3
- Some activities moved from grant to commercial licence income – grant support can leverage additional funding and activities

CCP-EM commercial income

- CCP-EM software suite licensed for a modest fee to for-profit organisations / activities
- Agreement to use this income for supporting further CCP-EM activities
- STFC finances
  - Ideally spend within FY, though some mechanisms to carry over
  - Follows CCP4 precedent
- Status
  - Beginning to get modest income stream, though not enough to fund full positions (cf CCP4)
  - Aiming to support training and short software projects

Commercial budget

Income *		
2018 / 2019	£4,691	
2019 / 2020	£60,002	
2020 / 2021	£50,098	So far …
Expenditure		
Spring Symposium April ‘19	£20,000	subsidy
EMBO course Sept ‘19	£3,000	sponsorship
GRS 2020	USD 2,000	Sponsorship (carried over)
Cowtan (York) – work on Gemmi library (10 weeks)	£18,000	Under negotiation
Topf (BBK) – work on TEMPy library (6 months, 50%)	£24,000	Under negotiation
Global Phasing / LMB project	TBD	Top-up funding

* Income apportioned to FY according to licence period

CCP-EM software suite

- See Agnel's talk from the Spring Symposium
  https://www.ccpem.ac.uk/downloads/symposium/AgnelJoseph_ccpem_symposium_2020.pdf
- Latest stable release is v1.4 from November 2019
- Later additions include cryoEF, SIDESPLITTER, Haruspex, difference map utility, EMDA
- Nightly build contains Relion 3.1
- https://www.ccpem.ac.uk/download.php

Workshops (since last report)

- 4 – 5 Sept 2019, Harwell, CCP-EM/CCP4 machine learning, 35 attendees
- 23 Jul 2019, SBGrid webinar series, demo of CCP-EM
- 2 – 12 Sept 2019 Birkbeck, EMBO cryoEM course, tutorial on CCP-EM
- 3 – 9 Nov 2019 Hamburg, EMBO integrative structural biology, talks / tutorials
- 7 – 9 Jan 2020, CCP4 Study Weekend on “Model Building and Beyond”, Alan Roseman co-organiser, Lunchtime Bytes on CCP-EM
- 23 Feb – 4 Mar 2020, Ben-Gurion University Israel, 2nd CCP4/BGU Workshop on Advanced Methods for Macromolecular Structure Determination, talks/tutorials

Spring Symposium

- 2020 location was switched to the East Midlands Conference Centre. More expensive but better catering! Used by the CCP4 Study Weekend.
- Clearly overtaken by events, but will be used in 2021.
- 2020 Online Spring Symposium. Over 3000 people registered. Around 1000 – 1200 attendees on Zoom at any one time.
- Talk slides available at https://www.ccpem.ac.uk/training/spring_symposium_2020/spring_symposium.php
- Likely to add Zoom element to 2021 meeting.
- Seeking scientific organisers for 2021.

Related projects

- Wellcome Trust validation grant (Peter Rosenthal)
  - Tools now appearing in CCP-EM suite
  - Model validation task, difference map utility, proshade, EMDA
  - End-of-grant conference planned for 2021
- Joint project between CCP-EM, Global Phasing and Sjors.
  - Funded by STFC Innovations, Global Phasing and CCP-EM
  - Just recruited person to work on software framework linking Relion, other CCP-EM software and Global Phasing software (e.g. Buster)
  - https://www.globalphasing.com/
- “A community-based training programme for CryoEM” recently funded by Wellcome Trust for Leeds/eBIC/Glasgow/Leicester
  - Coordinate closely with CCP-EM training schedule

Questions for community

- We are looking for small collaborative software development projects that are of benefit to the wider community and can be distributed through CCP-EM. We can potentially fund / co-fund these from our commercial licensing. Suggestions please!

- How can we encourage deposition of raw and intermediate data to EMPIAR?