MINUTES OF THE CCP STEERING PANEL MEETING
TUESDAY 5 DECEMBER 2017
JISC, LONDON

Attendees:

Adrian Mulholland, University of Bristol – Chair
Damian Jones, STFC – Secretary
David Brown, Kent – CCP4
Giovanni Ciccotti, Rome
Frances Collingborn, NERC
David Corney, STFC
Megan Dowie, MRC
Catherine Jones, STFC - SESC
Martin Lueders, STFC – CCPmag (*on behalf of J Staunton*)
Barbara Montanari, STFC
Stephen Perkins, UCL – CCP-SAS
Leon Petit, STFC – CCP9 (*on behalf of Mike Payne*)
Mark Savill, Cranfield University – CCPEngSci
Kris Thielemanns, UCL – CCPPetMR
Ilian Todorov, STFC – CCP5 (*on behalf of Neil Allan*)
Sue Thorne, STFC – Software Outlook
Phil Withers, Manchester University – CCPi
Scott Woodley, UCL – MCC Materials Chemistry
Graham Worth, UCL – CCPQ
Jonathan Yates, Oxford - CCP-NC

Apologies for Absence:

Neil Allan, University of Bristol – CCP5
Tony Arber, Warwick University – CCPP
Michael Ball, BBSRC
Chris Brown, JISC
Rachael Bruce, JISC
Deborah Greaves, Plymouth University – CCP-WSI
William McAllister, EPSRC
Luke Mason, STFC – Software Outlook
Mike Payne, Cambridge University – CCP9
Matt Probert, University of York – UKCP
Peter Rosenthal – CCPEM
Julie Staunton, Sheffield University – CCPmag
Geerten Vuister, Leicester University – CCPN
Martyn Winn, STFC – CCPEM

Adrian Mulholland welcomed everyone to the meeting.

1. Apologies for Absence

Apologies were as listed above.

2. Minutes of previous meeting (26 June 2017) and matters arising

The minutes of the previous meeting were approved with the following changes:

- CCP12 should be changed to CCPEngSci in all instances.
- The Software Outlook report needs more details – not just a list of bullet points.
- Adrian Mulholland should be listed as Chair not Chairman.
- In the NERC report on p3 the second sentence in the GCRF update should be removed as this item is currently under discussion.

Actions:

All CCP Chairs – CCP Chairs to pass on existing case studies and be aware that Marion O'Sullivan (Impact Manager, STFC) will be contacting people in the future. An external impact report has been commissioned by STFC and work will start this week. Case studies will be included. ACTION COMPLETE

Damian Jones – Invite Neil Chue-Hong to the next meeting to present on Software Accreditation League Table. Neil will speak today. ACTION COMPLETE

Erica Yang – Speak with Phil Withers to see if CCPi can do something around a joint biology conference with imaging or machine learning as a theme. Erica has not spoken to Phil about this yet but Phil confirms that he is happy to be involved and will coordinate with Erica. ACTION ONGOING

Barbara Montanari - Consider who we could approach from an industrial/commercial background to comment on CoSeC relaunch. CoSeC as launched officially at the RSE Conference in Manchester, September 2017. ACTION COMPLETE

3. Programme News from Research Councils

STFC – David Corney – The STFC e-leadership strategy has now been through a number of different levels of approval. It has progressed through the final level at Council and if approved will be released to the public in the New Year. Brian Bowsher is stepping down when UKRI is formed in 2018. Interviews have taken place for his replacement and his successor will be announced in January. CoSeC launched officially in September at the RSE Conference. Computing Insight UK will take place in December in Manchester with the theme of joining up the UK e-Infrastructure.

BBSRC – Michael Ball has been seconded to ESRC. His replacement has not responded.

NERC – Frances Collingborn – HPC:

- NERC has a high, and rising, over demand for HPC.
- Met Office collaboration: In addition to Monsoon2, which is a joint NERC/Met Office development platform for collaborating NERC/Met Office scientists, NERC has, since April 2017, a new HPC service 'NERC share of the XCS' (NEXCS). NEXCS is dedicated to NERC only use. In total for the two services, NERC buys into 8.4% of the Met Office's XCS (XC40). NEXCS provides NERC with about one third of NERC's current share on ARCHER. Initial uptake has been from the Atmospheric and Oceanographic consortia, with the Mineral and Geophysics consortia trialling users.
- The contracts for ARCHER, Monsoon2 and NEXCS all end in December 2018. NERC is currently considering the future split of the HPC recurrent budget.
- JASMIN: Capital was approved in 2017 for an upgrade to JASMIN. The initial concept was to provide data storage and analysis for Monsoon users, this has been widened to include more of NERC's remit. It is now possible to transfer data to JASMIN from NEXCS.
- Via the HPC application forms, we have been collecting publications and impacts generated from use of ARCHER/HECToR since 2009. Recently an analysis was done, which identified over 1,000 unique associations, more than 200 of which had not been captured by other methods (such as Researchfish). The overall NERC HPC citations impact was over 2, slightly higher than the NERC average.

Industrial Strategy Challenge Fund (ISCF) – NERC is participating in this activity via Robotics, Faraday batteries, and Medicines manufacturing. Other industrial priority areas are Sustainable food and Energy.

EPSRC – William McAllister – Not in attendance but sent a written report. Susan Morrell has confirmed that the next call for Tier2 RAPS is likely to be released in February 2018. Some proposals have been transferred from Tier2 to ARCHER. The procurement for ARCHER 2 is under way but the budget is not set yet. David Corney explained that Brian Bowsher has been asked by Mark Walport to lead on UKRI

Infrastructure. BEIS are starting to push towards the commercial cloud option but the scientific community is starting to push back against this. EPSRC are developing a call on centres for doctoral training to be released in January. Scott Woodley asked what happens to the CDTs when the funding runs out. They cannot continue in Universities that have no funding for them. Phil Withers highlighted that the subjects for the CDTs should be based on what the UK economy needs not just because they are "sexy" subjects. Adrian Mulholland mentioned the RSE model and asked if this is something that other councils may follow up on? Frances Collingborn confirmed that NERC have been approached with a view to providing funding but discussions are still ongoing. MRC currently accepts research fellows around priority subjects.

ESRC – Fiona Armstrong – not in attendance

MRC – Megan Dowie – *summary to follow*

JISC – Rachael Bruce – not in attendance

4. CoSeC (SLA) Steering Committee

Barbara Montanari spoke on behalf of Matt Probert.

The SLA has now been relaunched as CoSeC – as recommended by the Steering Committee – at the RSE Conference in September. There was an article in Research Fortnight following the launch. The EPSRC part of CoSeC will go through an International Review in 2018.
Barbara provided an explanation of the recent trend with regard to publications from CoSeC funded staff and made a request to CCP Chairs to include CoSeC staff as co-authors where relevant.

David Corney explained that with UKRI approaching fast we need to keep the momentum going with CoSeC now but we do not know who to raise this with at UKRI? Adrian Mulholland agreed to draft an email from all CCP Chairs to send to Rebecca Endean (Strategy Director for UK Research and Innovation) at UKRI. ACTION: Adrian Mulholland to draft an email on behalf of all CCP Chairs to push CoSeC with UKRI and circulate for comment.

5. Reports from the CCP Projects

The CCP reports were circulated before the meeting for information. Where Chairman were in attendance the following points were raised:

CCPBioSim – Adrian Mulholland – There has been recent cross CCP activity with CCP-EM and CCP5. Hannes Loeffler has left his post at STFC recently. Interviews have taken place and a replacement should be secured shortly.

CCPN – Geerten Vuister – no report.

CCP-NC – Jonathan Yates – Currently enjoying some industrial participation with a 1 year student placement (just completed 4 months at Astra Zeneca and is now at Johnson-Matthey). His job is to see if the software is being used correctly and if there are changes to be made. This arrangement is working very well. The ARCHER model doesn't work for the community but they have been able to join with UKCP and get access via that route.

CCP4 – David Brown – the current CCP4 grant includes some Cloud computing. Electron crystallography may form an aspect of the next grant proposal.

CCPEM – no representative.

CCP9 – Leon Petit – The flagship project is based on the Questaal code, a GW code that can scale up to 80 atoms. A recent training course was well received. Collaborating with Julie Staunton (Warwick) and AMES Lab in the States – and also currently starting a collaboration with Salford University. A new flagship on the Onetep code with Nick Hine is being developed and currently looking at opportunities to work with SuperStem at Daresbury.

CCPi – Phil Withers – The community is growing rapidly. Recent town meetings were well attended. The flagship started in April and they have had three papers accepted recently. Due to appoint a new recruit ASAP.

CCP5 – Ilian Todorov – A three day training course at QMUL in April with 20 participants and another one at Strathclyde in September at the back of the AGM with 15 participants. The summer school at Lancaster in July and the AGM at Strathclyde in September were delivered successfully. The school had 67 participants and AGM was attended by 87 delegates. The CCP5 Summer School will move from Lancaster to Durham for three years from 2019. The DL_MONTE flagship project had a 3 day splash event at Bath in April delivering training to 25 academics over 3 days. Drs. Ilian Todorov and Michael Seaton were successful in attracting H2020 funding, awarded in May 2017, for 2 PDRAs over 3 years to work on a software interoperability project, VIMMP, in the area of mesoscale and molecular modelling. On the UK side the project includes UNILEVER, IBM UK and University of Manchester.

CCPEngSci – Mark Savill – Consortia covered by CCPEngSci have all made renewal bids. UKAAC now has evidence to support its claim for more resources and will now move forward with a proposal.

CCP-SAS – Stephen Perkins – UK funding has finished but US funding carries on until next year. There is no longer a postdoc in the UK. Stephen went to India recently to give training courses as well as Pakistan to present on work. A number of grant applications are in the pipeline.

CCP-WSI – A number of meetings and workshops have taken place over the last six months. The 1st code developer's workshop was held in July as part of the OpenFOAM workshop in Exeter where 37 experts participated.

CCPQ – Graham Worth – The flagship project is starting with Queens Belfast and the Open University. CCPQ has encountered some problems with recruiting. Currently on their third round of interviews. Collaboration with ECAM is working well.

CCPPetMR – Kris Thielmans – *summary to follow*

CCPCDM – no representative.

CCPPlasma – no representative. Barbara Montanari reported that Joseph Parker has achieved some quite impressive speed up. Details are included in the CCPPlasma report.

CCPmag – Martin Lueders – have run under-staffed but are now looking to hire a postdoc for the next two years. The recruitment process is complete and an offer has been made, with the hope to start in the New Year.

Software Outlook – Sue Thorne – Currently looking at putting together training material for the code-coupling work. They can show a 15% saving on DL_POLY by using mixed precision. A software audit questionnaire is now complete and will be sent out next week. There have been some staffing issues but Xiahou Guo has now come on-board to provide extra effort.

SESC – Catherine Jones – Currently chasing account PIs to make sure they are still active PI's.

6. Presentation

Neil Chue Hong presented on the Software Accreditation League Table.
The slides can be found here https://doi.org/10.6084/m9.figshare.5669743.

7. Date of next Meeting

The next meeting will take place on Friday 8 June 2018 at the MRC, One Kemble Street, London.

Damian Jones
20 January 2018

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Action	Owner	Progress
Speak with Phil Withers to see if CCPi can do something around a joint biology conference with imaging or machine learning as a theme	Erica Yang	**Ongoing**
Draft an email on behalf of all CCP Chairs to push CoSeC with UKRI and circulate to CCPSP members for comment.	Adrian Mulholland	**New Action**