

# MINUTES OF THE CCP STEERING PANEL MEETING HELD ON MONDAY 26 JUNE 2017 MRC, KEMBLE STREET, LONDON

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## **Attendees:**

Adrian Mulholland, University of Bristol – Chairman  
Damian Jones, STFC – Secretary  
Tony Arber, Warwick University – CCPP  
Michael Ball, BBSRC  
Frances Collingborn, NERC  
David Corney, STFC  
Megan Dowie, MRC  
Katherine Freeman, EPSRC (*by phone*)  
Deborah Greaves, Plymouth University – CCP-WSI  
Catherine Jones, STFC  
William McAllister, EPSRC (*by phone*)  
Luke Mason, STFC  
Barbara Montanari, STFC  
Marion O’Sullivan, STFC  
Mike Payne, Cambridge University – CCP9  
Stephen Perkins, UCL – CCP-SAS  
Matt Probert, University of York – UKCP  
Andrew Reader, KCL – CCPPetMR  
Peter Rosenthal – CCPEM  
Mark Savill, Cranfield University – CCPEngSci  
Julie Staunton, Sheffield University – CCP Mag  
Kris Thielemans, UCL – CCPPetMR  
Ilian Todorov, STFC – CCP5 (*on behalf of Neil Allan*)  
Martyn Winn, STFC – CCPEM  
Scott Woodley, UCL – MCC Materials Chemistry  
Graham Worth, UCL – CCPQ  
Erica Yang, STFC – CCPi (*on behalf of Phil Withers*)

## **Apologies for Absence:**

Neil Allan, University of Bristol – CCP5  
Chris Brown, JISC  
Rachael Bruce, JISC  
Giovanni Ciccotti, Rome  
Geerten Vuister, Leicester University - CCPN  
Phil Withers, Manchester University – CCPi

Adrian Mulholland welcomed everyone to the meeting.

### **1. Apologies for Absence**

Apologies were as listed above.

### **2. Minutes of previous meeting (5 December 2016) and matters arising**

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

- Agenda Item 3 – NERC – should read “working with EPSRC on a replacement for ARCHER...”.
- Agenda Item 4 – SLA Steering Committee – should read “...panel members on an international review from outside the UK are ~~always jealous~~ envious of theCCPs...”.

Actions:

*Damian Jones - Invite Mike Brady to attend the next meeting and present.* Despite attempting to contact Mike Brady, Damian had been unable to complete the action at this point. If anybody has contact details for Mike please forward to Damian. ACTION ONGOING

*All Panel Members - Send suggestions for future external speakers to Damian.* ACTION ONGOING

*Damian Jones – Confirm our acceptance of the replacement RIKEN representative.* Damian completed this action by email following the last meeting however there has been no reply from the new representative in relation to his meeting. ACTION COMPLETE

*Damian Jones – Invite Happy Sithole to join the Steering Panel.* Happy has accepted our invitation to join the panel but was already booked for another meeting on this date. He will join for the December meeting. ACTION COMPLETE

*Damian Jones – Contact CCP4 and request attendance at the next meeting.* CCP4 have submitted a report for this meeting but were unable to attend. ACTION COMPLETE

### **3. Programme News from Research Councils**

**STFC** – David Corney – ELC is still expected to be set-up. The intent is still there. The General Election halted progress. BEIS sees ELC as an important group and there is lots of speculation about ELC membership and the Chair. Brian Bowsher is leading on the UKRI infrastructure group – more information will be provided on this in the future. STFC is close to finalising its e-Infrastructure strategy. The document is going to Science Board this week and Executive Board later this year. Mark Forster has now moved over to the Hartree Centre with Barbara Montanari now leading the applications division. The SLA between STFC and EPSRC is being renamed as CoSeC in an effort to raise the profile of the work. Marion O’Sullivan is the Impact Manager for CoSeC and is looking for stories that will showcase what the CCPs do. She is specifically looking for stories that have an effect on society and the economy, as well as stories that highlight impact for the end users. Marion will start with the CCPs covered by the SLA because of the mid-term International Review of the programme that is taking place next year but will have the scope to expand at a later date. Matt Probert mentioned that the HECs submit three case studies each year to the ARCHER web site that might be worth looking at. **ACTION: CCP Chairs to pass on existing case studies and be aware that Marion will be contacting people in the future.**

**BBSRC** – Michael Ball – highlighted machine learning within the biological sciences in recent responsive node. There was a very strong response. Related applications have been received (25) with various approaches to machine learning. They held a recent workshop with SSI and Elixir about distributing software and making software available and are now developing some guidance for applicants and reviewers. There is a joint activity with STFC under the Newton Call about data reuse in India around animal health – integrating data sets, enhancing data sets, and transforming data into something that is understandable to the end user. There is a £3m budget and this work should start moving forward at the end of this year / start of next year. Adrian highlighted that this is an area where cross-CCP activity could be encouraged and would be useful.

**NERC** – Frances Collingborn – Amber Vater is the new Head of NERC Science Facilities and Data, to include HPC and e-Infrastructure. The recommissioning of the five NERC data centres is ongoing and that of the NERC facilities is due to start. There will be a town meeting for the ARCHER 2 community on 12 July – invitations have been sent and attendees will be able to input their requirements. A questionnaire has been circulated for those that cannot attend, or people can email Katherine Freeman with input. NERC is re-organising the governance of HPC and will form a new strategic committee, which will meet annually and include members from the current steering committee. The latter will be able to focus more on allocations – there is currently a huge demand from the NERC community. NERC and Met Office have renewed the ongoing collaborative platform, Monsoon2. In addition, NERC has entered into a new agreement with the Met Office to purchase a dedicated NERC share of the Met Office's main supercomputer, the XCS (solely for NERC users). This is named 'NERC share of XCS or 'NEXCS'. The contracts for Monsoon2 and NEXCS will be signed imminently. NERC has also approved some extra capital for JASMIN.

**GCRF** – Some collective funds have been issued by RCUK. GCRF schemes administered and run by RCUK are not currently considered as RC money, as opposed to those run by individual councils. Applicants should include ARCHER usage details. Schemes are only available to UK applicants. NERC and EPSRC have developed some guidance, which is now with the GCRF team, and which will be made available on the ARCHER web site once approved.

**EPSRC** – Katherine Freeman – software had a fellowship call which is now closed. There is a panel meeting coming up with £4m available for between 4-8 fellows. EPSRC is revising its software strategy. A draft has been circulated to those that attended the workshop last year. They are revising the strategy based on comments received at the meeting. A final draft will be available on the EPSRC web site when people who did not attend the last meeting will be able to submit comments. EPSRC is trying to make the strategy wider based on feedback received. Adrian felt that a draft should be circulated before it is placed on the web rather than adding the draft to the website before it is finalised.

A call for access to all Tier-2 machines is being drafted now. This should go live in early August. The Materials Chemistry system will have a different access system through the consortium. For access to Cambridge Tier-2 consortia should contact Mike Payne for information about access. A consortia call is also out now for existing and new consortia, for an allocation on ARCHER and into ARCHER 2 as well.

Bill McAllister will be the new contact for the CCPs at EPSRC. Katherine will remain contact for the HECs. Phil will also be the EPSRC contact for CoSeC.

**ESRC** – Fiona Armstrong – not in attendance

**MRC** – Megan Dowie – The Skills Development Fellowship scheme has recently been revised, to include quantitative skills and support early stage research students. Now institutions apply directly to MRC for fellowships and then the institution will assign the fellowships – rather than potential fellows coming directly to MRC for interviews. The scheme is still open for applications. The Informatics Institute has been renamed Health Data Research UK and will be co-funded by the health research departments of England, Scotland and Wales, ESRC, EPSRC, Wellcome, and the British Heart Foundation. Some capital funding from BEIS has also been received for CCP-EM recently.

**JISC** – Rachael Bruce – not in attendance

ELC – Peter Coveney – not in attendance. Covered under STFC above.

#### 4. CoSeC (SLA) Steering Committee

Matt explained that it is acceptable to use a University PDRA to make up small shortfalls in manpower. Large shortfalls should always be a recruitment. Current work is being focussed around the international mid-term review that takes place next week. CoSeC was renewed last year for five years with condition that there was an International Review after two years. This will take place in 2018. There will be four or five people on the panel – one from the CoSeC Steering Committee, one from the EU, one from the States, one from Asia and an external commercial member. The review will aim to look at the historical work of the SLA and future direction, and whether value for money is achieved using the current model.

A five year financial model is in place which allows some flexibility to move effort around over the five year SLA cycle. There was a plea to CCP Chairs to consider whether it is relevant to include CoSeC staff on papers/publications if they have been involved in the work. The meeting had an update from SSI about the Software Accreditation league table. **ACTION: Invite Neil Chue-Hong to the next meeting to present on this.** There was also an update from SESC and Software Outlook.

#### 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 – contributed to the CCP5 Summer School, joint conference with CCPN, Sarah Harris presented in June at the CCP-SAS Workshop, and a CCP-EM training workshop in Leeds in July. The CCP multiscale conference will run again with CCP5 in early 2018.

Steve Perkins asked about the potential for a joint biology CCPs workshop. CCPBioSim and CCP9 would both be interested if somebody was to put together an over-arching “biology” workshop. A theme such as imaging or machine learning could work for a joint conference. **ACTION: Erica Yang will speak with Phil Withers to see if CCPi can do something around this.**

**CCPN** – Geerten Vuister (Adrian Mulholland spoke) – a new MRC grant started in this reporting period.

**CCP-NC** – Barbara Montanari – organised a joint workshop with UKCP last summer. Albert Bartock-Partay joined at STFC.

**CCP4** – Martyn Winn – currently have a work package looking at cloud computing, making CCP4 available via virtual machines and integrating with SCARF and DIAMOND. Looking to diversify the ways that people can run CCP4. There will be a separate work package looking at learning from the outputs and taking CCP4 towards machine learning. CCP4 will be 40 years old in 2019 – there will be an official function to mark this event and they have recently started discussions about how to approach it.

**CCPEM** – Peter Rosenthal – the Spring Symposium had two hundred attendees. A model building workshop was held in April.

**CCP9** – Mike Payne – a flagship application based around the ONETEP code was successful and a Young Researchers meeting took place in April. Mike announced that he will be stepping down as Chair of CCP9 in the next few months.

**CCPi** – Erica Yang – a code inventory review has taken place. The first release will be in the next few months. CCPi was successful with its flagship application. The community has grown around 10% which is a healthy growth. They have supported one H2020 bid and also support the TOSCA event. CCP-EM have a workshop early next year which presents a good opportunity for a cross-CCP project. Martyn and Erica will discuss.

**CCP5** – Ilian Todorov – held an industrialist meeting at DIAMOND last year with CCPBioSim involved. They are currently involved with lots of training including the CCP5 Summer School and DL\_SOFTWARE Workshops. There has been lots of recent interaction with MCC and CCPBioSim. CCP5 was successful in the last e-Infrastructure call. Matt asked if CCP5 is confident they can make up the effort shortfall accumulated over the last two years. Ilian explained that they have made two appointments instead of one and the flexibility allowed with the profiling allows them to make up over the next few years.

**CCP12** – Mark Savill – the CCP has now changed its name to CCPEngSci. EPSRC are keen for them to take on a wider remit than previously with CCP12. The work covers various HECs – UKTC, UKTRF, UK-COMES (which provides a link to CCP5 through DL\_FIELD and DL\_MESO). EPSRC are keen that they should cover structural and fluid – the coupling is covered by CCP-WSI and there is good interaction between the two.

**CCP-SAS** – Stephen Perkins – now in the last year of their grant which will finish in October. A paper was published last December to summarise the work of CCP-SAS. When the grant finishes the work won't stop because there are studentships in place. They are currently negotiating to renew the CCP but this is difficult because it covers such a wide area of subjects. There has been suggestion to split into a soft matter project and a biology project as that may be easier to manage. Each would aim for its own renewal. Training that is scheduled for India looks very much like a GCRF project.

**CCP-WSI** – Deborah Greaves (Catherine Jones spoke) – blind tests are scheduled. Full details are included in the CCP-WSI report.

**CCPQ** – Graham Worth – successful with their flagship proposal which will bring together two strands of code that have been moving apart over the last ten years. They have a joint workshop with CECAM later this year. Relationships with STFC are good.

**CCPPetMR** – Andrew Reader – the software framework is now called SIRF. This combines two packages – STIR and GADGETRON. Their flagship proposal was successful. Applicants for that post are now being shortlisted. Two students have been funded to go to France and Belgium. Andrew mentioned that a workshop on imaging (spatially-localised parameter estimation) would be of great interest to PetMR.

**CCPPlasma** – Tony Arber – Tony highlighted that the main obstacle for new people now is not learning the code (there is generally good documentation) but having the required computing skills needed. CCPPlasma is considering changing a workshop next year to a course to cover this.

**CCPmag** – Julie Staunton – the main obstacle for CCPmag at the moment is understaffing.

**SESC** – Catherine Jones – They received eighty five responses to their recent survey and that included developers funded by every research council. Currently SESC is focussing on looking at policy around active / not active projects.

## 6. Presentation

Luke Mason, STFC presented on the Software Outlook project. There were various points raised:

- Mark Savill – all looks good and is an improvement on the past. Training would be welcomed.
- Matt Probert – are we talking about just SLA funded CCPs, all CCPs or CCPs and HECs? Luke confirmed he is happy to be as broad as possible and include as much as possible.
- Adrian Mulholland – how do we show impact for the mid-term review? Luke confirmed that training is one way he hopes to do that. Monitoring metrics will be difficult but should be achievable.
- Adrian Mulholland – look at the working group members and identify which areas are covered and could there be more gender diversity? Luke confirmed that the members were suggested by the SLA Steering Committee originally. They are now looking at the term members should serve and how they should then be changed.

## 7. Any Other Business

- Frances Collingborn pointed out that the Monsoon service at the Met Office is only for collaborations with the Met Office. The new service NEXCS will not need a collaboration.
- Barbara Montanari – CoSeC relaunch – it was suggested by Susan Morell that CoSeC could be extended to include support for STFC staff funded by other research councils. The general feeling is this would be good. Adrian would like to think about including an industrial representative who would be able to comment on this type of thing. **ACTION: Barbara to consider who we could approach from an industrial/commercial background.**
- CCPCMC (CCPCompMedChem) – this is a new CCP. They have held two workshops at Diamond and Cambridge and are waiting to hear the outcome of a grant proposal submitted to innovate UK. Extra information is included as Appendix 1.

## 8. Date of next Meeting

The next meeting will take place on 5 December 2017 at JISC, London

*Damian Jones*

**21 July 2017**

**ACTIONS OF THE CCP STEERING PANEL MEETING  
HELD ON MONDAY 5 DECEMBER 2016  
STFC RUTHERFORD APPLETON LABORATORY**

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<b>Action</b>	<b>Owner</b>	<b>Progress</b>
Invite Mike Brady to attend the next meeting and present	Damian Jones	<b>Ongoing</b>
Send suggestions for future external speakers to Damian	All Panel Members	<b>Ongoing</b>
CCP Chairs to pass on existing case studies and be aware that Marion will be contacting people in the future	All Panel Members	<b>New Action</b>
Invite Neil Chue-Hong to the next meeting to present on Software Accreditation League Table	Damian Jones	<b>New Action</b>
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	<b>New Action</b>
Consider who we could approach from an industrial/commercial background to comment on CoSeC relaunch	Barbara Montanari	<b>New Action</b>

## **APPENDIX 1**

### **CCP CMC Overall Goal**

CCP CompMedChem - a CCP for *in silico* small molecule compound design. Built up of academic method developers, industrial CADD groups and software providers. Aimed at providing a route-to-use for computational methods, a portal for naive users to find best practice and ensuring novel methods are focussed on industrially relevant problems.

### **Headline Outcomes**

1. Two workshops held (Diamond and Cambridge and attended by over 20 people (details below)
2. £1.3 M grant proposal submitted (hear back next week)
3. Open-sourcing of the SQUONK platform and introduction of third party tools <https://squonk.it/> commitment to continue to do so
4. Third meeting being organised for October and training workshop to be held this year

### **Workshops**

Meeting March 10th: 18 Attendees from pharmaceutical industry, software providers, academia at Diamond Light Source

### **Summary**

In the morning, three core topics were discussed. 1) Is this a useful ambition and is there will in the room to proceed? 2) What are the short term (InnovateUK - deadline April 12th) and long term ambitions and what are people able to commit to? 3) What are the actions and the timelines?

In the afternoon we discussed the proposed technical setup in more detail and how CCP CompMedChem would fit into the framework of CCPs and STFC's strategic goals.

### **List of attendees**

At Diamond (18): Frank von Delft - DLS/SGC; Anthony Bradley - Oxford/DLS; Garrett Morris - Oxford; Tim Dudgeon - Informatics Matters; Will Pitt - UCB; Mike Bodkin - Evotec; Ben Allen - e-Therapeutics; Mark Forster - STFC; Nathan Brown - ICR; Martyn Winn - CCP4; Sameer Velankar - PDBe; Jason Cole - CCDC; Andrew Leach - ChEMBL; Oliver Smart - PDBe; Jonathan Hirst - U of Nottingham; Ian Wall - GSK; Paolo Tosco - Cresset; Illian Totrov - CCP5

Videoconference (4): Matthias Rarey - U of Hamburg; Marcus Gastreich - BioSolveIT; Val Gillet - U of Sheffield; Peter Schmidtke - Discngine

### **Outcomes**

1. CCP CompMedChem would be beneficial for all parties
2. Industrial parties were willing to contribute in-kind to grant applications. Academic parties were willing to contribute time and resources in adopting the platform and generating tools for it.
3. The InnovateUK application should be submitted and focussed on XChem problems.



Meeting June 21st: 21 Attendees from pharmaceutical industry, software providers, academia at the University of Cambridge

### **Summary**

In the morning the submitted InnovateUK application (£1.3M involving CCDC, GSK, IM and Diamond) was described, progress on the first CCP CMC project (SQUONK) was described. Including the open-sourcing of the codebase. A proposed hackathon / training program was presented. In the afternoon specific cutting edge problems were presented by GSK and IOTA scientists and discussed.

### **Outcomes**

1. A SQUONKathon should happen - focussed on engaging academics and consultants into incorporating tools into SQUONK to solve naive user problems
2. A further meeting should happen in the autumn focussed around the tools of the EBI and Andreas Bender (who will organise the agenda / speaker list)
3. Parties are willing to contribute project time (pharma) development time (academics) to resolve the issues highlighted in the meeting

### **List of attendees**

At Cambridge (21): Anthony Bradley - Oxford / DLS; Frank von Delft - SGC / DLS; Sam Hughes - AstraZeneca; Dave Clark - Charles Rivers; Jason Cole - CCDC; Tim Dudgeon - Informatics Matters; Ben Allen - eTherapeutics; Ian Wall - GSK; Will Pitt - UCB; Andrew Leach - ChEMBL; Nathan Brown - ICR; Garrett Morris - Oxford; Steve Roughley - Vernalis; John Hancock - Earlham/Elixir; Andreas Bender - Cambridge; Brian Marsden - Oxford; Paul Emsley - Coot/CCP4; John Overington - MD Catapult; David Bailey - IOTA; Fredrik Svensson - Cambridge

Videoconference (1): Val Gillet - U of Sheffield;