

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

Attendees:

Adrian Mulholland – Chairman
Damian Jones, STFC – Secretary
Jonathan Yates, CCP-NC
Mark Forster, STFC
Matt Probert, University of York – UKCP (*by phone*)
Mike Payne, Cambridge University – CCP9
Martin Turner, STFC (*on behalf of Phil Withers – CCPi*)
Neil Allan, University of Bristol – CCP5
Stephen Perkins, UCL – CCP-SAS
Kris Thielemans, UCL – CCPPetMR
Steve Linton, CCP CoDiMa (*by phone*)
Tony Arber, Warwick University – CCPP
Peter Rosenthal, - CCPEM
Katherine Freeman, EPSRC
Frances Collingborn, NERC
David Corney, STFC
Barbara Montanari, STFC
Catherine Jones, STFC (*on behalf of Deborah Greaves – CCP-WSI*)
Luke Mason, STFC
Mark Savill, Cranfield University – CCP12
Matt Probert, University of York – UKCP (*by phone*)
Bill Jones – UKCTRF (*on behalf of Nilanjan Chakraborty – CCP-WSI*)

Apologies for Absence:

Phil Withers, Manchester University – CCPi
Ryutaro Himeno, RIKEN
Deborah Greaves, Plymouth University – CCP-WSI
Graham Worth, UCL – CCPQ
Julie Staunton, Sheffield University – CCP Mag
Giovanni Ciccotti, Rome
Dominic Tildesley, CECAM
Megan Dowie, MRC
Michael Ball, BBSRC
Rachael Bruce, JISC
Richard Catlow, UCL – MCC Materials Chemistry
Scott Woodley, UCL – MCC Materials Chemistry
Nilanjan Chakraborty, Newcastle – UKCTRF
Geerten Vuister, Leicester University - CCPN

Adrian Mulholland welcomed everyone to the meeting. Mark Forster gave a quick description of his background and his new role within STFC as replacement to Paul Sherwood.

1. Apologies for Absence

Apologies were as listed above.

2. Minutes of previous meeting (24 June 2016) and matters arising

The minutes of the previous meeting were approved without changes.

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

Damian Jones - Update CCP website to show Adrian Mulholland as Chair. ACTION COMPLETE

All Panel Members - Send suggestions for future external speakers to Damian. Martin Turner suggested a presentation about the Tier 2 centres with information about how to get access etc. Further suggestions are welcome. ACTION ONGOING

3. Programme News from Research Councils

STFC – David Corney – pleased to welcome Mark Forster as the new Head of Applications Division and Deputy Director of the Scientific Computing Department. Brian Bowsher has been elected as the new head of STFC. A £20m proposal for the Ada Lovelace Centre has been submitted. Currently waiting for the outcome in the autumn statement.

BBSRC – Michael Ball – no report. Michael’s input to the last meeting was welcomed. Mike Payne asked if there was any cross-research council discussion between the council representatives? It was confirmed that there is an RCUK quarterly meeting and they do have conversations. **This panel would encourage input from all councils to this meeting. If a representative cannot attend then they should send input electronically or ask one of the other councils to represent them.**

NERC – Francis Collingborn – working on a replacement for ARCHER to come online in 2018. Looking to finalise a new contract with the Met Office, to commence on 1 April 2017. They are moving their systems onto the Exeter Science Park on 1 April.

EPSRC – Katherine Freeman – there were 17 proposals to the recent software call. The panel meets in January 2017. A software workshop was organised from which there was lots of feedback which will be compiled into a report and made available online. EPSRC is interested in having another RSE call but there is no budget yet. They have recently funded Edinburgh (standard x86 cluster), Midlands (standard x86 cluster), Bristol / GW4 (ARM architecture), Oxford (GPU cluster for machine learning), UCL (standard x86 cluster) and Cambridge (petaflop of x86, petaflop of knights landing, petaflop of GPU) Tier 2 centres. There will be an official launch event in Birmingham and invitations to this will be sent out.

ESRC – Fiona Armstrong – not in attendance

MRC – Megan Dowie – not in attendance

JISC – Rachael Bruce – not in attendance

ELC – Peter Coveney – not in attendance. Katherine Freeman spoke briefly. Mike Payne commented that ELC is not completely dead. David Corney read an email exchange between Tony Hey and Joe Johnson that confirmed this and invited discussion about future options. We should invite Tony Hey to keep us up to date about future plans and it is noted that this panel is happy to help.

Adrian requested again that for future meetings research councils should send input electronically if they cannot attend the meeting in person.

4. SLA Steering committee

Matt Probert updated the panel on the last SLA Steering Committee Meeting that was held in July 2016. This was also the last meeting for Paul Sherwood. The committee discussed the impact of the SLA work and how to circulate the information. They also discussed a new approach to handling any underspend. The SLA is now profiling resources over 5 years instead of 1 year. The SLA has been renewed. It was reported at the last CCP Steering Panel meeting as being renewed for 2 years which was not true. It has been renewed for 5 years with a review after 2 years. The review will be held in

the autumn 2018. The steering committee, STFC and EPSRC are currently looking at renaming the SLA and issuing a joint press notice to announce the new name.

The SESC/CCPForge activities were examined with a report provided from Catherine Jones. The steering committee were very pleased to see Luke Mason involved with Software Outlook and the advisory board for that project coming together. They are now creating a more concrete workplan and looking to progress in the future. The next meeting is scheduled for February 2017.

There was a brief discussion about the impact of the work completed within the SLA and in particular how it is defined and ultimately broadcast. Matt Probert pointed out that this helps to make a case for value for money of the SLA. Mike Payne pointed out that panel members on an international review from outside the UK are always jealous of the CCPs because they do not have a similar system, so panel members from outside the UK will be more appreciative.

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 – have recently organised a useful workshop with CCPN and a joint meeting with CCP5, plus a joint workshop with CCP5 at Diamond.

HECBioSim – Adrian Mulholland – the Longbow work is going well. One joint proposal with CCPBioSim was submitted under the flagship project. They have now received the referee's feedback.

UKCTRF – Prof W Jones – the project is working well. A 2-day workshop was held in Durham last September that was successful. A follow up meeting will be organised for this September. The main problem they have is a lack of time on ARCHER. They have applications for twice as much time as they have available. The majority of their people are doing DNS (Direct Numerical Simulations) and Large Eddy Simulations. DNS uses a lot of time. Large Eddy needs long run times.

CCPPetMR – Kris Thielemans – holding six weekly meetings with users / developers. Nearly all of the software is currently written by STFC staff but do have some PhD students that are now in a position to help. STFC staff visit universities to help with teaching. A flagship proposal was submitted and they are currently writing a response. There is a big emphasis from the community to have easy distribution. The first solution was to use a virtual machine with a virtual box but there was a bug that hindered this approach. Another problem was the use of Matlab but that can't be installed on a virtual machine. Now looking at Docker as a potential solution.

CCPi – Martin Turner – held their main TOSCA conference and also welcomed some summer students, one funded by STFC's Scientific Computing Department. Currently taking SAVU (Diamond) and using that as a framework instead of some of the other commercial offerings. They will have a new recruit starting soon.

CCP9 – Mike Payne – has a flagship project being run by Mark van Schifgaarde. Also applied to the recent software for the future call. A young researcher event was organised and CCP9 will also be having a community meeting next April. Support from Daresbury has been very good and very efficient.

CCP-SAS – Stephen Perkins – now in the last year of funding. This project receives joint funding from USA and UK. Making good progress with publications and posters. More people are using the software than ever before, mainly for biology work. A training course will be held in January at Coseners House. Stephen would be very interested in talking with CCPEM and CCPBioSim about potential joint working.

CCPEM – Peter Rosenthal – a developers workshop was held in October. There is potential for cross-collaboration with CCP4 and a big demand for training. There has been a rapid progression in the development of this project and as a result there is a requirement for a 1-day scoping workshop to help people understand what is needed by CCP-EM. Barbara Montanari mentioned the Ada Lovelace Centre as a potential collaboration with both CCP-EM and CCP-SAS.

CCP-WSI – Deborah Greaves (Catherine Jones spoke) – a focus group was held in the summer with over 50 academics that was very successful.

CCPQ – Graham Worth – making good progress and is currently focussed on three main codes.

CCPPlasma – Tony Arber – Joseph Parker is now working on magnetic codes and recently set-up collaboration with Oxford e-Science Research Centre, Culham and NAG.

CCP5 – Neil Allan – their recent annual meeting went well after initial problems with the original organisers and venues. This year the event included an industry day. The CCP5 Summer School at Lancaster was also a success. The new CCP5 website using Drupal is now live. It has been confirmed that accounts can be created for non-stfc staff for editing purposes – contact Damian Jones in the first instance.

CCP-NC – Jonathan Yates – organised the annual CASTEP training workshop in August 2016 – with focus sessions on CCP-NC software tools – and released the first public version of the “Soprano” software. CCP-NC has an open job advert to hire a widening participation PDRA who will work with key contacts to develop NMR Crystallography within Industry. An open call for interest was held last year, with the result that AstraZenica, Johnson-Matthey, The Cambridge Crystallographic Data Centre and Pfizer are our project partners. Pleased to welcome Albert Bartok-Partey to the team. Albert is developing machine learning approaches to the prediction of solid-state NMR parameters (which might also have interest to CCP5), and working on databases of NMR parameters (in partnership with CCP9).

Software Outlook – Luke Mason – the working group is now in place. Looking to improve the way software outlook interacts with the community and also looking to role out some webinar training courses with Labs to download. The courses will also be able to be presented at meetings and Universities in the future. Suggestions for potential topics should be sent to Luke. Currently looking at mixed precision – technical reports are about to be published and will be added to the web page. SLA funded CCPs should be able to provide suggestions. Mark Savill mentioned code_saturne and OpenFoam – Luke is already in contact with Dave Emerson.

SESC – Catherine Jones – the Build service is now in production. An informal technical network has been established. A survey was circulated and the response was good. There were users from all of the research councils represented. Next step is to investigate Matlab issues – Mike Payne can help with contact details.

CCP12 – Mark Savill – very active despite the fact they are not currently funded. They are looking at potential funding options. The EPSRC Infrastructure has been very helpful. They have been able to offer some assistance to allow important work to take place. CCP12 is looking to organise a Spring meeting.

CCP CoDiMa – Steve Linton — have published two minor releases of GAP (GAP 4.8.5 in September and GAP 4.8.6 in November 2016), and plan to make the next major release of GAP 4.9 available in 2017. SageMath released version 7.3 in August and 7.4 in October, including major additions such as [N. Cohen and D. V. Pasechnik. Implementing Brouwer's database of strongly regular graphs. CoDiMa funded further short collaborative visits. Markus Pfeiffer (St Andrews) visited Alan Logan (Glasgow) to work on the practical implementations of methods to compute with hyperbolic groups and Awss Al-Ogaidi (University of Sussex) visited St Andrews to work on parallelisation of the GAP code for a problem in finite geometry. Organised the 2nd CoDiMa Training School in Discrete Computational Mathematics in Edinburgh in October.

6. Presentation

Andrey Brukhno from STFC gave a presentation on the DL_MONTE package.

7. Global Challenges / GCRF

How do we engage with the global challenges agenda? The most fertile area is where we can provide expertise and input to projects. It is harder for us to engage as a community than for some other communities.

David Corney confirmed that STFC/SCD have a small team to look into GCRF and they are starting to formulate some bids now.

Frances Collingborn understands that most of the money is not new money but is re-badged money. The difficulty with training people in computational science activities in developing countries may be the lack of infrastructure.

Adrian Mulholland stressed the importance of building networks in developing countries to ensure that as well as us providing input we get something back as well.

8. Any Other Business

- International/external representation from RIKEN – the panel agreed to accept the suggestion made by Prof Ryutaro Himeno for the replacement representative from RIKEN. **ACTION: Damian to confirm by email.**

Following the earlier discussion about the GCRF there was also some debate about an external representative from a developing country. [NOTE: following this meeting Damian circulated a suggestion to invite Dr Happy Sithole Director, Center for High Performance Computing in South Africa. Following positive responses from a number of panel members who know Happy personally an invitation will be sent to join the panel] **ACTION: Damian to confirm by email.**

- HPC and Big Data Conference – Ilian Todorov (CCP5) had circulated an email requesting speakers at this event. It was agreed that it should be left to individual CCPs or research councils to suggest speakers if they want to.

- Closure of NSCCS – the service will close by the end of January. Are the training needs of this community being met? There is some training from CCP5, CCP9, CCPBioSim and so on but we may want to think about what we can offer in the future.
- Director of CECAM – Dominic Tildesley steps down at the end of the year. His successor is Professor Ignacio Pagonabarraga Mora. He is keen that the CCP Steering Panel and the CCPs and CECAM maintain their links moving forward. He will be invited to future meetings.
- CCP4 – it was again stressed that we would welcome CCP4 attendance and input to these meetings. **ACTION: Damian to contact CCP4 before next meeting to request a representative attends and that they submit a report.**

10. Date of next Meeting

The next meeting will take place on 26 June at MRC, 1 Kemble Street, London

Damian Jones
23 January 2017

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Action	Owner	Progress
Invite Mike Brady to attend the next meeting and present	Damian Jones	Ongoing
Send suggestions for future external speakers to Damian	All Panel Members	Ongoing
Confirm our acceptance of the replacement RIKEN representative	Damian Jones	New Action
Invite Happy Sithole to join the Steering Panel as an international representative	Damian Jones	New Action
Contact CCP4 before next meeting to request a representative attends and that they submit a report	Damian Jones	New Action