



**Computational Science Centre  
for Research Communities**

## **Town Hall Meeting**

**Monday 1 – Tuesday 2 July 2024**

**Manchester Marriott Hotel Piccadilly**



## CONTENTS

Foreword.....	2
Introduction .....	3
Summary .....	4
Day One .....	4
Day Two.....	5
Discussions and Outcomes .....	5
CoSeC Funding.....	5
Cross-Cutting Computational Research Topics .....	6
Working Across UKRI.....	7
Conclusions and Next Steps .....	8

### Foreword

The **Computational Science Centre** for Research Communities (CoSeC) is an integral and long-term activity within STFC’s Scientific Computing department. Recent investment into the Centre by the UKRI Digital Research Infrastructure (DRI) programme now allows it to further develop and grow into a national hub for Computational Research. This meeting represented the start of this, and I was delighted to see such an enthusiastic response from researchers across UKRI.



The value of meetings like this come from the interactions they enable, and it is fair to say the discussion that took place in Manchester were both insightful and meaningful. As a Centre, CoSeC has several clear priorities and objectives over the next 3 years, some are tangible, like ensuring UKRI’s research communities have the immediate funding to enable them to utilise the Collaborative Computational Project (CCP) networking approach effectively. Others need continuous discussion to make sure we get things right in the long-term, such as what the key cross-cutting topics for UK computational research are or how communities can be better enabled to work across the UK’s research landscape.

We have compiled some of the meeting’s major outputs, some will have practical value as new communities are proposed, some will help inform existing communities around topics and priorities to consider. The idea of the CCP has existed for over 5 decades and in that time has grown and evolved enormously. There is inherent value in the model, and I am excited to see how it can be propagated across new communities and become a widely recognised element of the UK’s DRI landscape in the years to come.

Dr Stephen Longshaw  
*UKRI STFC Scientific Computing, CoSeC Director*

## Introduction

Following investment into the [Computational Science Centre for Research Communities \(CoSeC\)](#) by [UKRI DRI](#), this meeting explored the [Collaborative Computational Project \(CCP\)](#) model as well as other collaborative community approaches that are at the heart of what CoSeC does and how we can both support and proliferate them across UKRI while building a cohesive computational research strategy within the UK's Digital Research Infrastructure landscape.

Detailed information was provided about practical aspects of the new UKRI DRI CoSeC investment such as our upcoming funding opportunities and new support activities as well as detailed engagement around the new set of cross-cutting capabilities we are building within the Centre.

The event brought together Chairs of existing communities, CoSeC technical staff, representatives from across UKRI and those who have been previously involved in CCP-like community activities and those who may be interested in engaging. We are looking to create new cross-UKRI communities that revolve around aspects of digital research and in particular building community activities around software and related activities.

### DAY 1 – Monday 1 July

<b>12:00 – 13:00</b>	<b>Arrival – lunch available</b>		
<b>13:00 – 15:00</b>	Welcome and Introduction UK DRI Introduction CoSeC Overview SCD Theme Descriptions Theme Leaders Panel Discussion	Stephen Longshaw Richard Gunn Stephen Longshaw Theme Leaders Theme Leaders	15 minutes 15 minutes 30 minutes 30 minutes 30 minutes
<b>15:00 – 15:30</b>	<b>Coffee Break</b>		
<b>15:30 – 15:45</b>	Overview of Funding Opportunities	Stephen Longshaw	15 minutes
<b>15:45 – 17:15</b>	Breakout Session 1 ( <i>Funding</i> ) Wrap up and Discussion / Feedback	All Attendees All Attendees	60 minutes 30 minutes
<b>18:00 – 20:00</b>	<b>Evening Meal</b>		

### DAY 2 – Tuesday 2 July

<b>09:00 – 09:30</b>	<b>Arrival – coffee available</b>		
<b>09:30 – 10:45</b>	Recap of Day 1 and Introduction to Day 2 – Initial Findings CCPs Across UKRI Questions	Stephen Longshaw  UKRI Council Representatives All Attendees	15 minutes  45 minutes 15 minutes
<b>10:45 – 11:00</b>	<b>Coffee Break</b>		
<b>11:00 – 11:30</b>	CCP Chair Presentation	Dr Ivo Tews – Chair of CCP4 ( <i>Protein Crystallography</i> )	30 minutes
<b>11:30 – 13:00</b>	Breakout Session 2 ( <i>AI etc</i> ) Wrap up and Discussion / Feedback	All Attendees All Attendees	60 minutes 30 minutes
<b>13:00 – 14:00</b>	<b>Lunch Break</b>		
<b>14:00 – 14:30</b>	CCP Chair Presentation	Prof Shuisheng He – Chair of CCPNTH ( <i>Nuclear Thermal Hydraulics</i> )	30 minutes
<b>14:30 – 14:45</b>	<b>Coffee Break</b>		
<b>14:45 – 15:45</b>	Breakout Session 3 ( <i>Cross UKRI</i> ) Wrap up and Discussion / Feedback	All Attendees All Attendees	30 minutes 30 minutes
<b>15:45 – 16:15</b>	Invited Presentation	Prof Davide Costanzo – CCPs and the particle physics community	30 minutes
<b>16:15 – 16:30</b>	Wrap up and close	Stephen Longshaw	15 minutes

## Summary

### Day One

The meeting began with a welcome and an overview of CoSeC by the CoSeC Director, Stephen Longshaw. This presentation set the scene for the following two days of presentations and discussions.



The Programme Director for Digital Research Infrastructure at UK Research and Innovation, Richard Gunn, provided a high-level introduction to the UK DRI programme focussing on some recent developments such as the DRI second phase portfolio announced in March, which included the launch of funding opportunities for Net-Zero DRI leadership and community building,

Research Technical Professional (RTP) support, and federation of compute services. The portfolio also included the first cross-UKRI “Access to HPC” call and the installation of Isambard 3 – UKRI’s first compute service funded through the DRI programme and accessible to all of UKRI’s communities.

The DRI strategy forward look includes four strands:

- Human DRI: ensuring that we maximise the opportunities to digitalise research and innovation by supporting the highly skilled DRI professionals that will enable us to build deep technical knowledge and empower a wider user base.
- Interconnected DRI: enabling transformative research and innovation through collaboration that delivers a strong economy and effective public services.
- FAIR DRI: enabling the UK’s researchers and innovators to contribute to an open, accessible and collaborative digital research landscape.
- Sustainable DRI: building an internationally competitive federated national resource that increases the productivity of researchers and innovators.

Over the next year the UK DRI programme will:

- Continue to work closely with DSIT to deliver major compute investment, including new compute access mechanisms for Isambard AI and DAWN.
- Develop the case for further phases of investment in the UKRI DRI programme: developing a ‘data as a service’ model for the UK community, sustaining and enhancing our large-scale compute system, and developing the underpinning tools, techniques, services and skills required for a secure, sustainable and collaborative DRI.
- Implement the development of a ‘statement of requirements’ process to contribute ideas for the development of our DRI.
- Establish a data working group to advise on the development of a framework for articulating and prioritising the requirements of DRI users and enablers of FAIR principles.
- Openly recruit a further cohort of AGD members.



Following Richard's presentation, the meeting heard from theme leaders within STFC's Scientific Computing Department including Computational Maths, Data Analysis, Systems Infrastructure, Open Science, Computational Engineering, Computational Materials and Molecular Science, and Computational Biology.

The final presentation on day one was an overview of upcoming CoSeC funding opportunities, including bridging funding for existing funded communities and separate funding for new communities, alongside a programme of investment in CoSeC Fellows and Placement opportunities.

## Day Two

The second day of the meeting began with a series of short presentations from a selection of the UK Research Council representatives in attendance including EPSRC, NERC and AHRC and a panel discussion that also involved representatives from BBSRC, STFC and MRC that provoked some interesting questions and discussion points around how the CCP model is viewed across the different Research Councils.



The meeting attendees were also very appreciative of the three invited presentations from Dr Ivo Tews (Chair of CCP4 in protein crystallography), Prof Shuisheng He (Chair of CCP NTH in nuclear thermal hydraulics), and Prof Davide Costanzo who presented on the CCPs and the particle physics community. These presentations provided some background to each of the scientific areas and also some context as to how the CCP model works in each area, and the benefits these communities have seen. The presenters were also very willing to share their experiences of working in the CCP environment.

## Discussions and Outcomes

A major part of the meeting were the breakout sessions that took place over the two days. This section of the report will summarise the discussions from those sessions and highlight the outcomes. The breakout sessions covered three topics:

1. CoSeC Funding
2. Cross-Cutting Computational Research Topics
3. Working Across UKRI

## CoSeC Funding

This session was split between groups containing members of currently funded, existing communities and those from potential new communities. **The groups containing members of existing communities** were tasked with exploring the complexities of applying for and utilising the upcoming UKRI DRI funding invitation and how this will work across the known thematic areas. This considered known high-level DRI requirements like GPU acceleration, use of AI, sustainable computing and quantum, as well as where overlaps exist, and they can be worked into plans. **Those from potential new communities** discussed their understanding of the CCP

model and CoSeC as presented so far, including the nature of the upcoming open call to create new communities as well as looking at ideas of how existing networks that aren't currently a CCP can utilise this opportunity to take it forward.

As a result of discussions between those from potential new communities a number of suggestions were put forward for scientific areas that could be explored including:

- a CCP around conservation heritage sites with the aim to capture digital data and combine with geological data that currently cannot be completed as data is incoherent and fragmented with no common standards.
- a CCP exploring plant biology focussed on genomics and bioinformatics of plants that would require the development of AI analytic tools, a data gathering platform, as well as support and training around the tools needed to analyse the data gathered.
- a CCP that could produce integrated modelling and simulation to understand the dynamics of air quality and to categorise and analyse output data.
- a CCP to understand and analyse over 700 Pb of data per year generated through the Square Kilometre Array (SKA) and develop general software and workflows related to radio astronomy.

Other potential topics and communities mentioned included:

- a lattice quantum field community
- cosmology-planetary simulation with DiRAC
- a community based around power system research
- volume electron microscopy
- quantum crystallography
- chemical processes in simulation
- mineral and geophysics

## Cross-Cutting Computational Research Topics

This session explored known cross-cutting topics derived from the UKRI DRI objectives such as AI, Heterogenous Computing (GPUs) plus Sustainable and Quantum Computing and Data Curation like Research Object Cataloguing. The aim of this session was to think about these topics at a high-level, rather than focussed on any one specific community with a goal to identify each thread through UKRI where there is a commonality in the form of computational research.

The general feeling coming out of the discussion groups was that heterogeneous computing is valuable to the communities but also challenging and time intensive. The aim is to make codes work on all GPUs, but lack of a standard method poses difficulties, and CPUs are still obviously necessary. There was also some feeling that communities should exercise caution when developing GPU codes to avoid future limitations, as technological landscapes can change in 5-10 years. There is also the need for guidance on aligning software with current and future hardware architectures, determining the best fit for applications, adapting codes accordingly, and training the code developers.

The discussions highlighted a varying level of exposure to AI across the communities. The general opinion was that AI could be integrated across all areas, but that CoSeC should

consider offering cross-CCP support for communities lagging in knowledge and experience to help them learn and catch up.

There was support for the continuation of a CCP in quantum with some breakout groups commenting that quantum computing is exciting, but not currently usable by their communities. It would be great to create a feedback mechanism to keep communities updated on quantum computing progress and involvement opportunities, and maybe establish a forum for presenting problems where quantum computing experts can help. It would be helpful if there is a way to keep CCPs updated on quantum computing progress, stages for involvement, application suitability, and cost-benefit ratio.

Discussions around data curation included questions about determining who will set data standards, ideally at an international level, not just in the UK, as well as the ability to train communities on using existing data infrastructure as well as developing their own. It was stressed that proper data use is essential to avoid wasting resources and ensure sustainability.

Sustainable computing was also discussed with communities seeking help to measure and optimize the energy use of a program and minimize energy intensive data transfers. A link between sustainability and data management was identified with a need for guidance on sustainable practices.

## Working Across UKRI

This session was focussed on the idea of computational research across UKRI, including topics related to computational research and how they relate to different councils within UKRI. Examples could include data curation topics such as Research Object Cataloguing or AI or topics like agent-based modelling. Groups were also asked to include a discussion about the perceived blockers for working cross-UKRI as a UK researcher and potential solutions.

All groups recognised the potential for collaborative joint projects and programmes across the Research Councils, but they currently struggle to see any clear strategies to demonstrate how this could be achieved. Scientific areas such as biology can seek funding from different research councils (BBSRC & MRC for applications and EPSRC for methodology and computation). There are no barriers for Biology in cross-council collaboration. However, there is an awareness of the need to tailor messages for different research council and panels. There is also a general feeling that the appropriate buzz phrases for securing funding calls are not always known.

Many University RSE groups have successfully reached out to different research groups within universities representing various councils. We can learn from their experiences to enhance our outreach efforts. Bringing in generic RSE staff for short-term assignments on a project is ineffective. Emphasized the need for staff with specific domain knowledge and the importance of building personal relationships for successful project outcomes. Effective knowledge exchange across different research councils is essential. Although this has not been well managed in the past, there is confidence that the CoSeC Programme Office will improve information dissemination across the different CCPs.

One breakout group had an in-depth discussion about interdisciplinary vs multi-council: there was a consensus that most future work should be interdisciplinary, even though some specific activities like data curation may remain within one single council due to practical reasons.

Data management across research councils were noted with a focus on a lack of standards. NERC was recognised for its well-defined data management processes, and it was noted that

we have the potential to learn from NERC's approach. Data produced or managed by EPSRC is not available in unusable or reusable form. It was emphasized that one entity's discarded data could be valuable for another, especially in the context of machine learning and that metadata is not a "one for all" solution. It must be customized to meet the specific needs of the audience, for example, AHRC need to catalogue data differently for the general public and for research purposes.

## Conclusions and Next Steps

This Town Hall meeting represented the start of a new chapter for CoSeC, it aimed to facilitate conversations around the software that drives computational research across UKRI. Ideas and outputs generated are provided in this document and will prove useful as we all move forward together to continue the growth and evolution of our computational research landscape.

New collaborative community ideas are identified, all of which have the potential to cross boundaries in terms of individual research areas. Similarly, the potential for cross-cutting topics like AI and heterogenous and GPU computing are considered. Emerging technologies like quantum computing are clearly highly relevant even at this stage within some research areas while others are only just starting to understand the potential, it is important that forums enabled by CoSeC provide the right exploration environment for this.

Over the coming six months there will be several key events related to CoSeC including the start of approximately twenty new CCP grants as well as the first intake for the CoSeC Fellowship programme. The CoSeC Community Forum series will also continue, with at least two per year and the Centre's annual conference will run again in 2024 in Manchester as part of the wider UKRI STFC organised Computing Insight UK event.

Alongside this, CoSeC will be working hard to ensure it is building up the skills and people needed to support the CCPs and other collaborative communities in their computational research aims. Utilising outputs of events like this one as we go, will help ensure the resultant capability within the Centre is indeed one of national value.

A key question that now needs to be explored by those who champion DRI across UKRI's councils and within UKRI itself is what the next two years should lead to in terms of how CCPs and networking activities like them are viewed strategically. Their value and importance is clear, so now it is key to understand what method of support (both in terms of infrastructure and funding) should UKRI provide to ensure that they are stable, active and inherently useful for UK research and innovation. This will be looked at proactively by CoSeC, in collaboration with colleagues from across UKRI.





**Computational Science Centre  
for Research Communities**

Report produced by Damian Jones

## **Science and Technology Facilities Council**

Rutherford Appleton Laboratory,  
Harwell Campus, Didcot, Oxfordshire OX11 0QX, UK  
T: +44 (0)1235 445000 F: +44 (0)1235 445808

**Sci-Tech Daresbury,**  
Daresbury, Warrington, Cheshire, WA4 4AD, UK  
T: +44 (0) 1925 603000 F: +44 (0) 1925 603100

## **Contacts**

**Damian Jones, Programme Office Manager**

**Georgia Lomas, Events Manager**

CoSeC@stfc.ac.uk