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CoSeC 2026 Mid-Year Forum Report

Warwick Conference Centre, UK
3rd-4th June 2026

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July 2026

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CoSeC

Science and Technology Facilities Council

Scientific Computing

Computational Science Centre for Research Communities

Community Forum

Wednesday 3 and Thursday 4 June 2026

Warwick Conference Centre

Foreword

The UK High Performance Computing community is widely admired internationally for its high degree of coordination and resulting impact. Collaborative Computational Projects have existed for more than 40 years, complemented in recent years by High End Computing Consortia and now a wider range of other Network activities. Such successful open collaboration remains key to maintaining, further strengthening and building on UK leadership at the cutting edge of current HPC research; particularly as developments move at pace in AI and Quantum Computing as well as established digital simulation.

The original CCP Steering Panel of HPC community leaders and Research Council representatives has accordingly expanded into a wider Forum embracing all UK existing and new HPC communities to ensure most effective sharing of information, skills and insights amongst these and right across UKRI. This latest Forum Report again attempts to capture important emerging points in a succinct fashion to inform a wider audience so that the collective impact of contributions from the gathered experts and inputs from CoSeC can be maximised.

The Warwick Forum was the first to adopt a new two-day format. Day 1 followed the form of previous Forum events - allowing community chairs to receive latest information directly from all UKRI Research Council representatives, DRI, SSI and CoSeC, while directly feeding back, as well as discussing the developing Forum issues, community aspirations, and priorities for effective future funding given the new compute resource support landscape. Day 2 opened up a wider community interplay focused around key cross-cutting activities with valuable direct polling of opinions, feedback and information alongside specific discussions.

The Forum welcomed the new format, and funding development intentions, whilst recognising that strong investment s in software and data services remain as important as those rolled out for the compute hardware roadmap.

Prof. Mark Savill
Chair of CoSeC Community Forum

Introduction

The CoSeC Community Forum is a biannual meeting for the communities directly involved in the CoSeC programme. This includes the Collaborative Computational Projects (CCPs), High-End Computing Consortia (HECs), and representatives from across the UKRI research councils.

The Forum provides an opportunity for these communities to report on recent activity, explore future opportunities and discuss national strategy relating to computational research. It also supports networking, knowledge exchange and the sharing of good practice, while helping to identify opportunities for future cross-community projects.

New two-day format

The June 2026 Forum was the first to use a new two-day format.

Day 1: Strategic updates and community discussion

Day 1 followed the Forum's established format and was attended by CCP and HEC Chairs, together with representatives from UKRI and the research councils. The programme included a presentation from David Lusher, the 2025 CoSeC Impact Award winner from JAXA, alongside an important update from UKRI DRI and the UKRI communities. This update introduced the background to the proposed Community Centres of Excellence (CCEs) and National Computing Resources (NCRs).

Day 2: Cross-cutting technical themes

Day 2 was open to the wider CoSeC communities and focused on four themes identified by the CoSeC External Advisory Board:

- Energy Efficient Compute
- FAIR Data
- Artificial Intelligence
- Quantum Computing

Each theme was led by a session lead and included a mixture of presentations and open discussion.

The two-day format was well received by the communities, with the discussion sessions proving particularly lively and engaging. This report summarises the key updates, discussions and outcomes from the Forum.

Agenda

Day 1 – Wednesday 3 June 2026

09:30	**Arrival – refreshments and pastries available**	
10:00	Welcome	Mark Savill (Cranfield University)
10:10	Minutes (November 2025) and matters arising	Mark Savill (Cranfield University)
10:30	CoSeC Update	Stephen Longshaw (UKRI-STFC)
11:15	**Break**	
11:30	CoSeC Impact Award Winner 2025	David Lusher (JAXA)
12:00	UKRI Council DRI Session	UKRI Council Representatives
12:45	**Lunch and Poster Session**	
14:00	UKRI DRI Update and UKRI Communities To include a presentation on the Computational Centres of Excellence	Ben Yarnall (UKRI)
15:15	**Break**	
15:30	Introduction to forum discussion	Damian Jones (UKRI-STFC)
15:45	Forum Discussion: 1. CoSeC next phase proposal 2. Grand challenges linked to the industrial strategy and UKRI compute resources	ALL - See attached guidance notes for further information We will allow 30mins discussion for topic 1 and 20mins for topic 2, followed by 10mins for feedback in the form of 1min lightning presentations
16:45	Any other business, wrap up and day 1 close	Mark Savill (Cranfield University)
17:00	**Free Time**	
18:00	**Evening Meal at Warwick Conference Centre**	

Day 2 – Thursday 4 June 2026

09:30	**Arrival – refreshments and pastries available**	
10:00	Welcome and introduction to the day	Mark Savill (Cranfield University)
10:15	**Energy Efficient Compute (inc. GPU)** Session Lead: Jessica Huntley	This session will include a series of short talks showcasing views from different communities followed by a feedback session and interactive poll. The aim of the session is to motivate the embedding of energy efficient computing best practices across CoSeC communities, highlight existing work across CCPs and gather feedback on barriers and challenges.
11:15	**Break**	
11:30	**FAIR Data** Session Lead: Elizabeth Newbold	This session will include presentations from three CoSeC communities about their experience of FAIR data plus an open discussion and a conclusion that looks at "What CoSeC can do to help you on your FAIR journey".
12:30	**Lunch and Poster Session**	
14:00	**AI** Session Lead: Jeyan Thiyagalingam	This session will explore how AI is used across the communities with a series of presentations from communities with differing levels of experience of AI. The session will also include an open panel discussion.
15:00	**Break**	
15:15	**Quantum Computing** Session Lead: Paolo Trevisanutto	This session will provide an introduction to quantum computing with three presentations based around current work and a Q&A session. This session will also provide an introduction to the separate Quantum Algorithms Day on Friday.
16:50	Wrap Up and Close	Mark Savill (Cranfield University)

Summary

The CoSeC Community Forum was held at Warwick Conferences in June 2026, adopting a new two-day format for the first time following feedback from the previous Forum. Advice from the CoSeC External Advisory Board meeting held in March 2026 also helped shape the main technical themes for Day 2. The event brought together representatives from across the computational science landscape to discuss strategic developments, future priorities and areas of shared interest for the UK's computational research communities.

The revised format attracted strong participation both in person and online, reflecting the level of interest in CoSeC's future direction and the wider changes across the Digital Research Infrastructure landscape.

Day 1 followed the Forum's established strategic format, with contributions from UKRI research council representatives, CCP and HEC Chairs, CoSeC staff and invited speakers.

Day 2 opened participation to the wider computational research communities and focused on technical sessions covering Energy Efficient Computing, FAIR Data, Artificial Intelligence and Quantum Computing.

Key Updates

Day 1

Day 1 brought together CCP and HEC Chairs, UKRI research council representatives, CoSeC staff and invited speakers to discuss current activity, emerging opportunities and developments in the DRI landscape.

The programme included an update from CoSeC on current work across the communities, including technical activity, cross-cutting projects, the CoSeC Fellowship programme and the NPRAISE programme. Updates highlighted examples of community software development, GPU acceleration, AI and machine learning activity, the CoSeC catalogue, energy efficient computing, the recent NPRAISE call, and opportunities for communities to contribute to the CoSeC blog. The session also introduced CoSeC's proposed next phase, which would build on its long-standing technical support role while strengthening its ability to bring communities together around shared research and computational challenges linked to national priorities and societal impact.

A key feature of the day was the UKRI DRI update on the future national compute ecosystem, including the Next National Supercomputing Service (NNSS), National Compute Resources (NCRs), the AI Research Resource (AIRR) and the proposed Community Centres of Excellence (CCEs). The update followed the UKRI Compute Ecosystem Town Hall held the previous day and gave Forum participants the opportunity to discuss how these changes may affect existing and emerging communities.

In response to UKRI DRI's questions on Community Centres of Excellence, breakout discussions highlighted the need for clear access routes, transparent allocation criteria,

practical onboarding support, training, software expertise and guidance on how CCPs, HECs and other community structures might relate to future CCEs. Participants also emphasised that national compute provision should be treated as a wider support ecosystem, not simply as access to hardware.

The day also included updates from UKRI research councils on priorities, funding activity and emerging areas of interest, including DRI priorities, compute transition planning, research data policy, AI, trusted research environments, innovation pathways and research infrastructure. These updates were complemented by the 2025 CoSeC Impact Award presentation on OpenSBLI. Overall, Day 1 gave the community a timely opportunity to discuss major DRI developments, contribute feedback on CCEs, and take part in a structured discussion on CoSeC's proposed next phase and its contribution to the UKRI ASCEND process.

Day 2

Day 2 marked the first wider technical day within the new Forum format, opening participation beyond the usual CCP and HEC Chairs to the broader CoSeC computational research communities. It focused on four cross-cutting themes: **Energy Efficient Computing, FAIR Data, Artificial Intelligence and Quantum Computing.**

The sessions showed that communities are already engaging with these areas, with discussions covering sustainability and carbon reporting, FAIR data and software practices, AI adoption and validation, and the current opportunities and limitations of quantum computing. They also highlighted common needs around training, guidance, software and data infrastructure, sustainability, validation and responsible adoption of emerging technologies.

Across the day, participants identified a role for CoSeC in supporting cross-community learning, sharing good practice and helping communities respond to technical challenges that cut across individual CCP and HEC boundaries.

UKRI DRI discussion on Community Centres of Excellence (CCEs)

As part of the Day 1 UKRI DRI session, participants took part in a DRI-led discussion on the proposed Community Centres of Excellence. The questions focused on where CCEs could help address community challenges, how new or emerging software communities should be supported, where centralised support is most valuable, what good or excellent support should look like, and what incentives encourage participation in community-led initiatives.

Feedback showed that communities welcomed the opportunity to discuss the model but needed greater clarity on whether CCEs would act mainly as funding routes, access routes or broader support structures. Participants were concerned about how CCPs, HECs, CoSeC and future CCEs would fit together, and whether software development, training, skills, RSE support and community activity not directly linked to NCR access would still be supported.

Several groups also raised concerns about the short timeline for CCE development, particularly in the context of the ARCHER2 transition and uncertainty over future compute access. Suggestions included allowing more time for communities to develop strong proposals, considering bridging funding for CCPs and HECs during the transition, and designing CCEs flexibly enough to support activities that may not sit naturally within traditional grant models.

The discussion also reinforced the value of CoSeC's cross-community role. Participants highlighted CoSeC's capacity to support RSEs and RTPs, provide cataloguing and training expertise, coordinate across communities and help avoid gaps or duplication. Incentives for participation were linked not only to compute access, but also to software development support, training, best practice, community visibility and opportunities for researchers to share knowledge back into their communities.

Forum Discussion

The separate Forum discussion focused on CoSeC's proposed next phase and how its role could evolve within the changing UKRI DRI landscape. Participants considered the benefits and risks of CoSeC moving from a mainly technical support model towards a broader role in bringing communities together around Grand Challenge research, national priorities and future compute provision.

Overall, there was support for CoSeC taking on a stronger coordinating role, particularly where it can help connect communities, reduce duplication, advocate for computational science and help researchers navigate an increasingly complex DRI landscape. However, participants were clear that this should not replace the existing community-led model. The value of CoSeC's current relationship with CCPs and HECs, including access to technical expertise, RSE support, training, software development and trusted community structures, was strongly emphasised.

A consistent message was that CoSeC should help communities explain and connect their priorities with UKRI, DRI and Industrial Strategy objectives, rather than define those priorities on their behalf. Several groups described CoSeC as a potential "glue" or conduit between communities, councils, DRI, government and wider partners. This role was seen as particularly valuable in identifying common technical needs, sharing good practice, supporting new or emerging communities and helping community-led challenges connect to national opportunities.

Key themes from the discussion

1. CoSeC as coordinator, connector and advocate

Participants felt that CoSeC has a clear role in helping to connect communities, councils, DRI activity and wider partners. Several groups described CoSeC as the "glue" between CCPs, HECs, DRI projects and other initiatives, helping to reduce duplication and improve coordination across a complex funding and infrastructure landscape. Practical examples included coordinating information about multiple calls, providing a regular newsfeed of

upcoming opportunities through community mailing lists, and helping communities understand where their work fits within UKRI and Industrial Strategy priorities.

2. Preserving the bottom-up, community-led model

A strong theme was that CoSeC should support communities in defining and explaining Grand Challenges, rather than defining those challenges centrally and cascading them down. Participants valued the current bottom-up model, particularly the flexibility it provides and the access communities have to CoSeC's technical expertise and RSE support. Written feedback noted the importance of preserving the "RSEs as a service" model and warned that a more top-down approach could risk losing this flexibility or weakening the trusted partnership between CoSeC and the communities.

3. Aligning Grand Challenges with national priorities

Groups recognised the need to connect community-led challenges to national priorities, including the UK Industrial Strategy (IS-8), UKRI priorities and the future national compute ecosystem. However, they emphasised that communities are often best placed to explain how their domain-specific research contributes to those wider priorities. CoSeC could help by drawing out these links, identifying common technical connections between communities and supporting a clearer narrative for funders, government and wider stakeholders. Examples raised in the submissions included offshore wind as an obvious link for CCP-WSI and antimicrobial resistance as a potential way for biological communities to connect their work to the infectious disease challenge.

4. Recognising technical and compute challenges in their own right

Participants noted that not all communities will map neatly onto the proposed research Grand Challenges. The computing challenges identified in the proposal, including AI, FAIR data, accelerated compute, mixed precision and energy efficient computing, were therefore seen as important routes for engagement in their own right. These areas can cut across multiple domains and may provide a way for communities whose research does not sit naturally under a single national challenge to contribute to shared outcomes. Mixed precision was highlighted as an example of a technical development whose outputs and opportunities may need to be shared across several research areas, rather than remaining within one domain.

5. Navigation, onboarding and practical support

There was strong support for CoSeC acting as a navigation point for the DRI and national compute landscape, especially for new or emerging communities. Participants highlighted the need for clear signposting, onboarding materials, training resources, examples of successful applications, "show-and-tell" sessions and guidance on how to access and use national compute resources. Specific examples included the need for a central repository of training resources for national DRI, practical examples of "ideal" AIRR or national compute applications, and guidance to help communities understand access routes across AIRR, HPC and NCR systems. This was seen as particularly important where communities face "unknown unknowns" or have limited experience with national DRI provision.

6. Industry, wider partnerships and the role of an honest broker

Alignment with the Industrial Strategy was recognised as likely to increase the need for industry engagement. Participants noted that collaboration with multiple industry partners can be challenging, particularly where data sharing, commercial sensitivity or competing interests are involved. CoSeC was suggested as a possible "honest broker" that could help convene partners, support trusted collaboration and represent community needs in discussions with industry and other external stakeholders, especially where companies may be reluctant to share data directly with one another.

7. Communicating impact and making the case for investment

Participants emphasised the importance of communicating the value of computational science, research software, technical expertise and national compute infrastructure more clearly. CoSeC was seen as having a role in helping communities demonstrate how discoveries translate into impacts, particularly where those impacts are long-term or difficult to measure. The submissions noted that making the case for the next national supercomputer may depend less on measuring immediate research outputs and more on telling a convincing story about the value of high-performance computing, software, people and infrastructure. Participants also highlighted the need for stronger examples of how discovery research leads to impact, including examples that move beyond familiar cases such as the internet or GPS.

Several areas were identified as needing further clarification. These included the meaning of "wider partnerships", how Grand Challenges relate to NNSS priorities and existing community Grand Challenges, how communities and infrastructures such as DiRAC and PPAN-related compute should fit within the wider landscape, and how access to software environments and national resources will be managed. Participants also asked whether CoSeC was being asked to help shape national DRI Grand Challenges or to help communities align their technical work with them. Other practical concerns included the need for guidance through application "hoops", possible meta-allocation roles, clearer feedback on unsuccessful applications, and the risk of siloed compute access where AIRR, HPC and NCR resources require separate routes or are restricted to specific types of work.

Overall, the discussion indicated that the community sees CoSeC's next phase as an opportunity to strengthen coordination, advocacy and strategic alignment, provided that this builds on, rather than replaces, the existing community-led model. The feedback also highlighted that future success would depend on practical support, clear routes through the DRI landscape, sustained technical expertise and continued openness between CoSeC and the communities as national priorities and compute infrastructure evolve.

Cross-cutting Technical Themes

1. Energy Efficient Compute – Led by Adam Greenbank

The session opened with an overview of CoSeC's cross-cutting green-computing work. It aimed to raise awareness of current activity, highlight practical examples from different communities and identify barriers to wider adoption through Q&A and poll feedback. The session included two talks designed to illustrate practical approaches from different areas:

- **Mariam Demir (CCP-EM) – *Biting back against carbon emissions: reducing our footprint in bioimaging***, which considered ways to reduce emissions across bioimaging workflows, including data collection, processing, compression and storage.
- **David McDonagh (CCP4) – *Sustainability in CCP4: Green DiSC and making software dynamic***, which shared CCP4's experience of Green DiSC certification and explored how software could become more adaptive and efficient over time.

The poll gathered 26 responses from across the CoSeC communities. It suggested growing awareness of green computing concepts, but less evidence of widespread practical adoption. Key barriers included lack of time, funding and incentives, alongside limited access to easy-to-use tools for measuring energy use and carbon emissions. Some respondents noted that HPC allocation models may not always encourage efficient resource use, as underusing allocations can affect future awards. Just under half of respondents had previous involvement in sustainability-related projects, most of which were performance-focused, with improved efficiency as a secondary benefit.

The Q&A focused on practical challenges and possible routes to greater efficiency. Discussion covered the role of data compression, whether optimisation should sit with users or facilities, how far lossy compression can reduce storage needs without compromising scientific quality, and decisions around older or less efficient equipment.

Participants also discussed the value of sustainability frameworks such as Green DiSC and how to evaluate whether adaptive software improves outcomes compared with existing workflows. The wider discussion explored the challenge of translating energy use into carbon emissions data, and whether carbon reporting would influence behaviour unless users were also given clear, practical options for reducing emissions. Participants also discussed whether future national compute infrastructure, including NCRs and the next national supercomputing service, should be expected or required to provide robust sustainability reporting as part of their service requirements.

The discussion suggested that CoSeC could support communities by sharing practical examples, improving access to measurement guidance and tools, and raising community needs in wider discussions about future compute infrastructure and sustainability reporting.

2. FAIR Data – Led by Elizabeth Newbold

The FAIR Data session explored how CoSeC communities understand and implement FAIR principles and what support may be needed. The session considered both FAIR data and FAIR software, recognising that findability, accessibility, interoperability and reusability are important across computational science but can mean different things in different communities. It was also emphasised that FAIR does not necessarily mean open, as access may need to be managed through licences, permissions or other safeguards. The session included three talks:

- **Wendi Liu (CCP-WSI) – *FAIR in the WSI community***, on how the CAT-WSI catalogue helps a multidisciplinary community find and access data, software, training materials and other resources, while highlighting challenges around large-scale data hosting, curation, funding and keeping resources up to date.
- **Wei Wang (CCP-NTH) – *Nuclear thermal hydraulics data and FAIR principles***, on applying FAIR principles in the nuclear thermal hydraulics community, using the RVACS benchmark case to make simulation results easier to compare, reproduce and reuse.

- **Sarah Harris (CCP-BioSim) – *FAIR in BioSim***, on the challenges of sharing large biomolecular simulation trajectories and workflows, and the need for well-maintained software, sustainable storage and data-sharing infrastructure, community trust and long-term commitment to make them reusable and reproducible.

The session used poll questions to prompt discussion. The first poll showed that FAIR is widely recognised but not fully embedded; 50% of respondents said FAIR was only somewhat supported or implemented in their community, while 41% said it was recognised but still challenging.

The second poll suggested that communities are generally strongest on making outputs findable and accessible, while interoperability and reusability remain harder to achieve. The discussion highlighted that reusable data and software need clear documentation, well-recorded workflows and agreed terminology, especially where communities use different terms for similar things. Participants also discussed the role of AI in helping to find and reuse data and software, noting that this depends on outputs being findable, accessible, well documented and supported by clear metadata. Community culture and trust were recurring themes, including how to encourage researchers to deposit data and software, how to give appropriate credit and how to ensure repositories, catalogues and software remain sustainable over time.

The final poll asked what would help communities make further progress. Responses highlighted the need for long-term infrastructure, funding for data curation and software maintenance, common templates, and clearer guidance on metadata, documentation, software sustainability and credit for shared outputs.

The discussion highlighted several ways CoSeC could help, including sharing good practice, supporting catalogue and metadata approaches, helping communities address storage and sustainability challenges, and advocating for funding models that recognise the ongoing effort needed to make FAIR work in practice.

3. Artificial Intelligence (AI) – Led by Jeyan Thiyagalingam

The AI session opened with a short overview of the rapidly changing AI landscape, noting that AI is increasingly being used not only for individual tasks, but as part of wider research and software workflows. The session then explored how AI is being used across communities, with examples from communities at different stages of adoption. It aimed to gather feedback on current use, training needs and community concerns, including trust, evaluation, human oversight, sustainability and the implications of AI tools for training and skills development. The presentation slides provide further detail on the individual talks, which ranged from arts, humanities and culture through to materials modelling and wave-structure interaction. Together, these examples showed that communities are engaging with AI in different ways and at different levels of maturity. The session included talks from three community perspectives:

- **Eamonn Bell (CCP-AHC) – *AI for Arts, Humanities and Culture in CCP-AHC***
- **Alin Marin-Elena (CCP5) – *AI for Materials and Molecular Modelling***
- **Yiyun Tan (CCP-WSI) – *Physics Informed Neural Operators***

The poll questions explored participants' views on AI tools, training needs and areas of concern. The first poll showed that participants were cautious about using results produced by AI agents. Of the 26 respondents, 46% said they would check everything an agent produces, while another 46% said they would trust low-risk outputs but would still verify anything important. Only 8% said they would spot-check the output rather than review it closely, and no respondents said they would mostly or completely trust an agent-produced result without checking. This suggests that, although there is clear interest in AI tools, people still see checking, validation and human oversight as essential.

The training poll showed strong interest in practical support. Training needs focused strongly on coding agents, prompting, evaluation, responsible use and good software practice such as version control, documentation and testing.

The open question to the panel and the Q&A raised several recurring concerns. Participants asked about the energy and carbon cost of AI tools, who is responsible for that cost, and how it could be measured. There were also questions about the ethics and legality of AI-generated code, including possible licence issues, how AI tools should be acknowledged in research outputs, and how PhD students and junior researchers can develop experience if routine "starter tasks" are increasingly automated.

The discussion also reinforced the need for clear safeguards, traceability and testing, especially where AI outputs could influence scientific conclusions, software quality or research integrity. A clear theme from the session was that AI is already becoming part of community research practice, but that its wider use will need to be supported by practical training, clear expectations and robust ways of checking and evaluating outputs.

4. Quantum Computing – Led by Paolo Trevisanutto

The Quantum Computing session provided an overview of current CoSeC and CCP-QC activities and explored where quantum computing may become relevant to CoSeC communities. The discussion focused on the practical question of what quantum computing might offer, what stage the technology is currently at, and how communities should prepare. The session included three talks, with further detail available in the presentation slides:

- **Martin Plummer –** ***Current CoSeC activities for CCP-QC: a quick round-up***
- **Scott Woodley –** ***presentation on quantum approaches for materials modelling***
- **Zhengliang Liu –** ***A Quantum Lattice Boltzmann Method based on Linear Equilibrium Distribution Functions***

The Q&A focused mainly on when quantum approaches might become practically useful compared with classical methods. Participants asked whether the examples shown were already faster on quantum hardware, whether current limitations are mainly about speed or scale, and what developments would be needed before quantum methods provide a clear advantage.

The discussion suggested that quantum computing is not yet a general replacement for classical HPC. Some approaches are still at the proof-of-concept or validation stage, and broader use will depend on more capable hardware, better ways of mapping problems onto

quantum systems, and effective hybrid workflows that combine quantum and classical computing.

There was also discussion of how quantum technologies may develop over the coming years. Participants noted that current machines remain limited, but that the field is developing quickly, with possible opportunities emerging over the next several years in areas such as materials, chemistry and biomolecular simulation.

In summary, the session suggested that not every CoSeC community needs to engage with quantum computing immediately, but that selected communities should continue to explore it now through proof-of-concept studies, shared learning and cross-community exchange. This would help identify where quantum approaches may become useful as the field develops, while being realistic about the current stage of the technology.

Conclusions and Next Steps

This Forum represented the first of a new two-day format designed following community feedback. The first day focussed on high-level strategy and future road mapping while the second provided a deep dive into four key thematic areas worked on across the communities and championed by CoSeC. I personally found this highly effective as it meant we could maintain the important community-led discussions recent Forum events have enabled while adding back in the technical flavour our meetings had in the past. This new approach will see a shorter, online meeting later in the year instead of a second in-person event, assuming that this is also seen favourably then we will look to keep this format in subsequent years.

In my conclusion of the November 2025 Forum I talked about the moving landscape for computational research introduced by UKRI's shift away from council-led infrastructure to a central approach there to deliver for all its research areas. In November, a major topic of conversation was around how we would manage access to the new National Compute Resources (NCRs) given that this is key part of the HEC model and a significant mechanism used by the CCPs where such access is required. As of this Forum, the six new NCRs were announced and a strong vision for the Next National Supercomputing Service (NNSS) also well understood.

A few days earlier, the UKRI DRI Programme held its own Town Hall meeting where they revealed the concept of the CCE (Computational Centre of Excellence) with a view to them issuing a call in Autumn 2026. These CCEs are expected to form part of UKRI's access mechanism for their new landscape of computing resources and so, understandably were a hot topic at this Forum. We were joined by UKRI's Ben Yarnall, as well as DRI colleagues from EPSRC who enabled a discussion session around the DRI programme's plans, CCEs and how the existing CCP and HEC community landscape might map into it. More detail can be found earlier in this report on what was discussed but the summary is that the DRI's approach to CCEs sees them fulfil multiple purposes, the communities themselves were unable to comment too much on whether the idea behind them was appropriate for their needs until more detail was released by UKRI about the number it intends to fund and what it will expect of them in terms of outputs and outcomes.

My own CoSeC update provided technical insight into work done across the communities as well as an overview of the projects being run centrally within CoSeC. These include a project around energy efficient computing and another that looks to enable FAIR and AI insight for the research object outputs of the communities in the form of the CoSeC Catalogue, with an initial prototype due in Winder 2026. I spent the remainder of my presentation describing a possible future model for CoSeC as we look to evolve along with the overall UKRI approach to DRI.

This new way of working sees CoSeC build on its 2025-2026 Grand Challenges to become a point of coordination for delivery against new UKRI-owned Grand Challenges as drivers for use of its computing infrastructure. These may be research or digital in nature and would allow the diverse, domain-specific landscape of CCPs and HECs to be convened thematically by CoSeC to deliver against these challenges. A longer discussion session around this idea was held later in the day and the outputs from that can be seen earlier in this report. Consensus was that the idea was sensible but there were differing responses from community Chairs around who is

better placed to lead on delivery of research grand challenges. I will now integrate this feedback into ongoing design discussions around a future CoSeC.

It is worth taking a moment to acknowledge that the entire funding landscape for CCPs and HECs has an imminent cliff-edge of March 2027. This is the same position that the majority of UKRI's computing infrastructure found itself in recently and is now being resolved by the delivery of the NCRs and NNSS. There is clear recognition within UKRI that research software is key to a successful DRI and therefore it must now rapidly put a strong, forward-thinking, structure around this.

As part of this, I will be using the outcomes of this Forum to create a strong proposition for what Research Software as an Infrastructure actually looks like within a national DRI and where CoSeC fits within that. What is clear already is that the grass-roots community approach the UK has evolved over decades is the envy of much of the world and a key asset for us to build a strong future on.

This Forum ended at a point of uncertainty in terms of the future for the entire community landscape. We saw clear messaging around current thinking within UKRI in terms of CCEs and how it wants to utilise its new computing infrastructure to deliver Grand Challenge research. It is now imperative that we quickly describe what this means in practical terms, so forward planning can begin in earnest across all communities.

I personally see great opportunity; the UK has built its own stable network of researcher-driven computational communities that self-organise the maintenance and ownership of key researcher codes and the infrastructure they demand. If this is effectively combined with a new mission-led approach that speaks to the Government's Industrial Strategy, then we will find ourselves in a truly world-leading position in terms of how we treat Research Software.

Dr Stephen Longshaw
Director of CoSeC

Appendix

CCP REPORTS

Materials Science

CCP-NC for the Period 01/10/25 to 31/03/26

Prof. Paul Hodgkinson (CCP-NC Chair), Dr. J. Kane Shenton (STFC Core Support)

1. Background

No changes to previous.

2. Outputs

During this reporting period, CCP-NC has continued to deliver against its workplan in the areas of machine learning, FAIR data, accelerated computing and community development.

A major milestone has been the continued development of the CCP-NC computational solid-state NMR database schema and associated software ecosystem. Building on the initial release of the schema package, we have worked closely with partners including the Physical Sciences Data Infrastructure (PSDI), NOMAD Laboratory, and developers of the CASTEP and Quantum ESPRESSO codes. This work establishes common standards for representing NMR tensors and metadata, enabling computational NMR data to be deposited, shared and reused in a FAIR-compliant manner.

Soprano, our Python library for NMR crystallography, has seen three further releases. Version v0.11.0 introduced a pluggable symmetry backend system, allowing Soprano to use either the established spglib library or the new Rust-based moyopy package, which offers improved performance and easier installation on some platforms. This release also fixed a long-standing correctness issue in unique-site labelling for structures in non-standard cell settings, and restored compatibility with SciPy 1.15. Version v0.11.1 improved compatibility with environments such as Pyodide (which allows Python scripting to be run within a web browser environment).

MagresView-2, our browser-based visualisation tool for NMR data, has also seen significant development activity. Version v0.2.0 added support for the extxyz file format, enabling visualisation of NMR data generated by machine learning tools (such as ShiftML), and improved maintainability through automated testing and dependency management. Version v0.3.0 overhauled the 1D plotting system to use the Plotly library, improving interactivity and user experience, and introduced keyboard shortcuts with an accompanying help interface. These releases were underpinned by several updates to the underlying CrystVis-JS visualisation library: improved extxyz handling, support for parsing and visualising hyperfine tensors from legacy magres blocks, an expanded camera and lifecycle API, and migration to the updated ESM/TypeScript-based crystcif-parse package.

CCP-NC has continued its programme of machine learning projects across two key strands: the use of machine-learned interatomic potentials (MLIPs) to accelerate structure sampling and molecular dynamics, and the development of neural network models to predict full NMR shielding tensors directly from structure. A highlight of this work is an end-to-end workflow developed in collaboration with external industry partners to predict NMR spectra for the industrially relevant zeolite STA-30, in which foundation MLIPs were used to generate structural ensembles and graph neural network models were trained on a DFT-computed subset to enable rapid spectrum prediction across a range of compositions. These approaches reduce reliance on computationally expensive density functional theory calculations, decreasing both time-to-science and the carbon footprint of large-scale studies.

In accelerated computing, work has largely been completed on migrating CASTEP's GPU implementation from the vendor-specific OpenACC programming model to the more portable OpenMP offloading standard. This transition is strategically important because OpenMP is supported across a wider range of compilers and hardware platforms, making the codebase substantially more vendor agnostic and reducing the maintenance burden associated with supporting multiple accelerator technologies. Benchmarking of the new implementation indicates that the performance benefits achieved with the original OpenACC port can be retained.

Community engagement has remained strong. The first CCP-NC Town Hall meeting, held in June 2025, kicked off the development of the community roadmap and strengthened engagement with early-career researchers through the formation of a dedicated early-career subgroup. The outline roadmap was recently reviewed by the CCP-NC Steering Group.

3. Research Implications and Impact

The outputs from this reporting period strengthen the technical foundations needed to make computational NMR crystallography more accessible, efficient and sustainable.

The development of standardised schemas, NOMAD integration and structured deposition infrastructure represents a significant step towards FAIR data practices in computational NMR. By enabling reproducible sharing and discovery of simulation results, these efforts allow for the creation of curated datasets that amplify the long-term value of community-generated data, particularly as training sets for machine learning models.

Advances in Soprano and related software infrastructure provide interoperable workflows linking density functional theory, machine learning and spin simulation. Ongoing maintenance ensures that Soprano remains robust and easy to install across the range of computing environments used by the community, including emerging platforms such as Pyodide. MagresView-2 complements this by providing an accessible, browser-based interface for exploring NMR datasets, with recent additions including support for ShiftML-generated extxyz files and an overhauled interactive plotting interface, lowering the barrier to visualising and interpreting results without any local software installation.

The machine learning projects directly address one of the community's major challenges: extending NMR crystallography to larger, more disordered and more dynamic systems. The zeolite workflow described above exemplifies this: by combining foundation MLIPs with

targeted DFT calculations and tensor prediction, it enables rapid, accurate spectrum prediction for realistic disordered catalyst models that would otherwise be computationally prohibitive. This has direct relevance to UK priorities in advanced materials and sustainable manufacturing as identified in the Industrial Strategy.

GPU acceleration of CASTEP will further reduce computational costs and energy consumption, support greener research practices while enable faster turnaround for complex calculations. Together, these outputs position CCP-NC to deliver substantial scientific and economic impact through accelerated materials discovery and more efficient use of national HPC resources.

4. Up to 5 research outputs that create an impact story for your community

1. Computational Solid-State NMR Schema and NOMAD Integration

Development of a standard schema for NMR tensor data, together with a NOMAD parser and structured deposition infrastructure, provides a FAIR foundation for sharing, curating and reusing computational NMR datasets. An initial deployable deposition and search infrastructure for curated magres datasets is planned for September 2026, enabling community testing and further population of ML-ready NMR datasets. The resulting data collections will have the necessary meta-data to serve as high-quality training sets for machine learning models, directly enabling the ML workflows described below.

2. Machine Learning Workflow for Predicting NMR Spectra of Defective Zeolites

In collaboration with a major international company, we have developed an end-to-end machine learning workflow to predict NMR spectra for the industrially relevant zeolite STA-30 across a range of Si:Al ratios. Foundation machine-learned interatomic potentials were first used to generate ensembles of low-energy defect structures efficiently. Density functional theory calculations were then performed on a representative subset of these structures to compute NMR parameters, which were used to train graph neural network models to predict full magnetic shielding tensors. The trained models were able to accurately reproduce DFT results for other Si:Al ratio structures, enabling rapid prediction of ensemble-averaged spectra, which would be impossible using traditional DFT-based approaches.

This workflow provides a practical route to the rapid prediction of NMR spectra for realistic models of disordered zeolite catalysts, accelerating the interpretation of experimental data and supporting the design and optimisation of industrially relevant materials. By October 2026, this work will be published as a citeable document either on our website or as an academic publication.

5. Workshops and new opportunities*

Date	Title	Description
29th June – 1st July 2026	CCP-NC NMR/ML Masterclass	Three-day advanced training course in Oxford covering GIPAW theory for solid-state NMR, efficient use of parallel HPC systems, visualisation and post-processing tools, and

		machine learning of NMR tensors. The course includes extended practical sessions where participants work on their own projects with feedback from tutors, as well as short research presentations. Targeted at researchers with prior experience of GIPAW.
TBC	CCP-NC Online	Our online lunchtime discussion seminar series. The planned CCP-NC Online Seminar series will cover a broad range of topics in computational solid-state NMR, including practical use of CCP-NC software tools, machine learning approaches for predicting NMR observables, paramagnetic NMR calculations, crystal structure searching, and methods for treating compositional and structural disorder. Additional proposed themes include modelling dynamics in NMR crystallography, nucleus-independent chemical shifts in solid-state materials, and industrial applications of NMR crystallography, with contributions from partners in the pharmaceutical and catalyst sectors. The series is intended to provide both technical training and a forum for discussion of emerging methodologies and applications across the community.

6. Issues and problems*

There has been some impact of the continued restrictions on core staff support, but we have responded creatively to the evolving circumstances and have continued to make steady progress on all our key objectives.

CCP5 for the Period 01/10/25 to 31/03/26

Prof. Paola Carbone, Prof Chris Lorenz (CCP5 Co-Chairs)

1. Background

CCP5 is the Collaborative Computational Project for computer simulation of condensed phase materials at length scales spanning from atomistic to mesoscopic levels. Founded more than 40 years ago, CCP5 has promoted the involvement of UK scientists in collaborative research achieved via software and methodology development, training, networking and outreach. It provides support for all UK scientists engaged in developing, applying and exploiting computer simulation methods for condensed matter systems. CCP5 has over 1500 UK and international members, which comprise research active academic faculty staff in 35 different UK universities and at least 18 other UK industrial, charitable or government organisations. A distinctive feature of CCP5 is its successful strategy of developing and disseminating new codes and methods for all kinds of materials problems. These include solid-state materials, polymers, colloidal solutions, liquids and mixtures, liquid crystals, surfaces and interfaces, homogeneous and heterogeneous catalysts, mineral, bio-mineral, organic and bio-molecular systems.

2. Outputs

CCP5 Undergraduate Bursaries
The CCP5 Summer Bursary is a competitive funding scheme run by CCP5 to financially support undergraduate students carrying out computational research projects over the summer, under the supervision of a UK academic. The following applicants were successfully awarded summer bursaries:

Marco Molinari (University of Huddersfield)
Chris Lorenz (King's College London)
Carla de Tomas (King's College London)
Ioan-Bogdan Magdau (Newcastle University)
Mark Miller (Durham University)
David Wales (University of Cambridge)

International Bursary exchange
This scheme supports PhD students based in the UK to visit international collaborators.

- **Gregor J. Lauter** University of Birmingham visit to the University of Toronto, support: £3,500
- **Ariel (Zac) Candelaria,** University of Edinburgh visit Exchange visit to University of Freiberg, support £850

Community workshops sponsored by CCP5

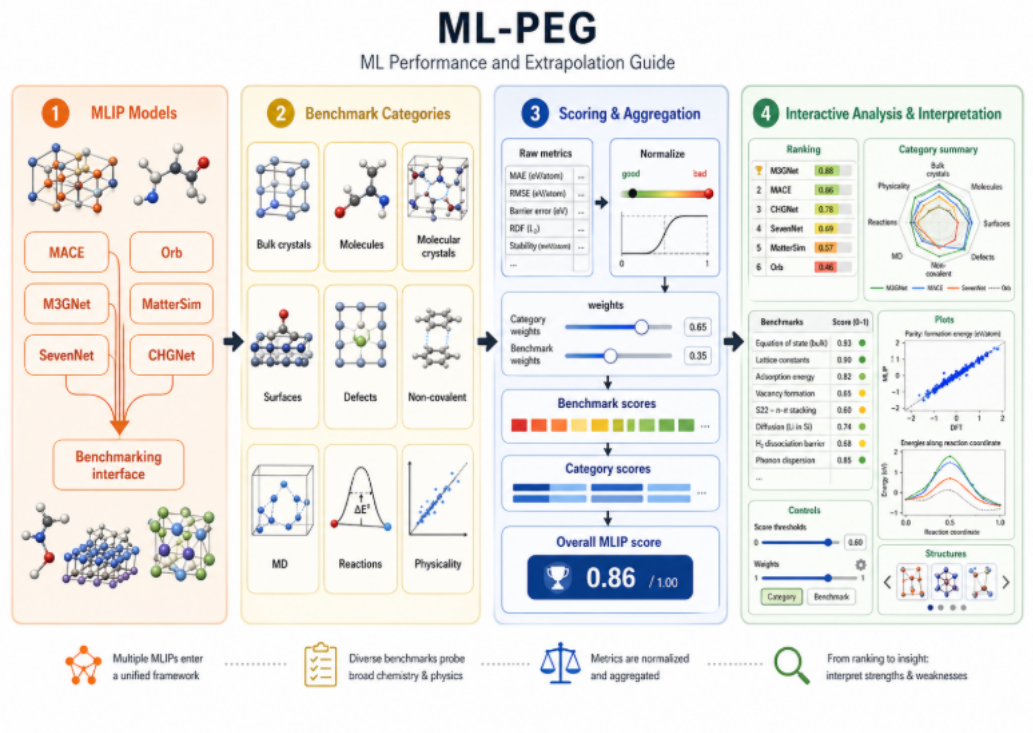
Molecular Modelling

- **Organiser:** Jochen Blumberger (UCL)
- **Event:** 20th anniversary symposium of the Thomas Young Centre
- **Support from CCP5: £1,000 (partial support approved)**

Data Science and Machine Learning for Polymer Physics

- **Organiser:** Daniel Read (University of Leeds)
- **Type:** One-day scientific workshop aligned with a CECAM event
- **Support from CCP5: £500**

Machine Learnt Interatomic Potentials Performance and Extrapolation Guide is a community effort lead by Alin Elena and Elliott Kasoar(lead developer, and part time PhD student at University of Cambridge, in Prof Gábor Csányi Group) that bring over 50 groups together from both UK and abroad to provide a reproducible and transparent framework for benchmarking and validation of foundation models. This aligns with the CCP5 working on bringing MLIPs to the community.



Publications:
Three publications result in the last period covering classical molecular dynamics, and AI:

1. H. Devereux, C. Cockrell, A. Elena, I. Bush, A. B. G. Chalk, J. Madge, I. Scivetti, J. Wilkins, I. Todorov, W. Smith, and K. Trachenko, “DL_POLY 5: calculation of system properties on the fly for very large systems via massive parallelism”, Computer Physics Communications 323, 110128 (2026).

2. I. Batatia, C. Lin, J. Hart, E. Kasoar, A. M. Elena, S. W. Norwood, T. Wolf, and G. Csányi, “Cross learning between electronic structure theories for unifying molecular, surface, and inorganic crystal foundation force fields”, arXiv preprint arXiv:2510.25380 (2025).

3. I. Batatia, W. J. Baldwin, D. Kuryla, J. Hart, E. Kasoar, A. M. Elena, H. Moore, M. J. Gawkowski, B. X. Shi, V. Kapil, P. Kourtis, I.-B. Magdău, and G. Csányi, “Mace-polar-1: a polarisable electrostatic foundation model for molecular chemistry”, arXiv preprint arXiv:2602.19411 (2026).

4. janus_core our MLIP code had a new release, code is used by more than 15 groups around UK and Internationally as a quick entry into the world of MLIPs.
5. ML-PEG, Machine Learnt Interatomic Potentials Performance and Extrapolation Guide went live. ml-peg.stfc.ac.uk

3. Research Implications and Impact

The three outputs detailed in Section 2 represent a paradigm shift in computational materials and molecular science, seamlessly bridging the gap between massive-scale classical simulations and highly accurate quantum methods. Collectively, they address core community Grand Challenges—specifically, working towards exascale computational readiness and deploying universal foundational AI models for chemistry and materials discovery.

The release of DL_POLY 5 (Output 1) tackles the critical Grand Challenge of scaling atomistic simulations to realistic, macroscopic dimensions. By enabling the on-the-fly calculation of properties for massively parallelized systems, researchers can now model complex microstructures, grain boundaries, and multi-phase interfaces—phenomena that dictate real-world material failure and performance but were previously computationally intractable.

Complementing this scale, the MACE foundation models (Outputs 2 and 3) resolve the historical trade-off between simulation speed and quantum-level accuracy. The development of MACE-MP (unifying molecular, surface, and inorganic models) and MACE-polar-1 (introducing polarisable electrostatics) democratizes access to state-of-the-art Machine Learning Interatomic Potentials (MLIPs). The real-world outcome is a drastically accelerated R&D pipeline: researchers can now perform highly accurate, predictive screenings of complex systems in a fraction of the time traditionally required by density functional theory (DFT). More importantly the MACE work was highlighted in the AI for Science Government strategy published on 20 November 2025, https://www.gov.uk/government/publications/ai-for-science-strategy/ai-for-science-strategy

4. Up to 5 research outputs that create an impact story for your community

1. H. Devereux, C. Cockrell, A. Elena, I. Bush, A. B. G. Chalk, J. Madge, I. Scivetti, J. Wilkins, I. Todorov, W. Smith, and K. Trachenko, “DL_POLY 5: calculation of system properties on the fly for very large systems via massive parallelism”, Computer Physics Communications 323, 110128 (2026).

2. I. Batatia, C. Lin, J. Hart, E. Kasoar, A. M. Elena, S. W. Norwood, T. Wolf, and G. Csányi, “Cross learning between electronic structure theories for unifying molecular, surface, and inorganic crystal foundation force fields”, arXiv preprint arXiv:2510.25380 (2025).

3. I. Batatia, W. J. Baldwin, D. Kuryla, J. Hart, E. Kasoar, A. M. Elena, H. Moore, M. J. Gawkowski, B. X. Shi, V. Kapil, P. Kourtis, I.-B. Magdău, and G. Csányi, “Mace-polar-1: a polarisable electrostatic foundation model for molecular chemistry”, arXiv preprint arXiv:2602.19411 (2026).
4. janus_core our MLIP code had a new release, code is used by more than 15 groups around UK and Internationally as a quick entry into the world of MLIPs.
5. ML-PEG, Machine Learnt Interatomic Potentials Performance and Extrapolation Guide went live. ml-peg.stfc.ac.uk

5. Workshops and new opportunities*

2026 Chemical and Materials Machine Learning School (CaMML), is a five-day intensive training event scheduled for April 13–17, 2026, at the STFC Daresbury Laboratory, Sponsored by CECAM, ALCHEMI, PSDI, PsiK, CCP5 and CCP9 (42 participants).

The CCP5 Summer School 2026, held at Newcastle University from July 19–30, 2026, serves as a premier training ground for the next generation of computational molecular scientists. This intensive two-week program provides early-career researchers with deep technical expertise in advanced simulation techniques, ranging from fundamental statistical mechanics and molecular dynamics to state-of-the-art machine learning interatomic potentials. Through a rigorous schedule of expert-led lectures and hands-on workshops, participants gain practical experience in the latest software workflows, fostering the high-level computational skills necessary to address complex challenges in modern chemistry and materials physics. Sponsored by CCP5, CECAM, CCP9, BioSim and UKCOMES. (around 70 participants)

The CCP5 Annual General Meeting (AGM 46), taking place from September 9–11, 2026, at the University of Edinburgh, serves as a vital focal point for the computational molecular science community. This gathering brings together researchers to review the latest developments in condensed phase molecular simulation, discuss the strategic direction of the community, and foster new collaborations. Through a blend of plenary talks and technical sessions, the meeting provides a platform for both established experts and early-career scientists to share cutting-edge research, debate emerging computational methodologies, and address the future challenges facing the field within the UK and beyond.

6. Issues and problems*

Lack of clarity in funding for next cycle creates uneasiness in the community around being able to continue the training and networking activities.

CCP9 for the Period 01/10/25 to 31/03/26

Prof. Stewart Clark (CCP9 Chair)

1. Background

No changes to previous.

2. Outputs

Up to a page detailing significant outputs for the period. Examples include details of work related to important topics such as accelerated computing, developments or applications of AI, quantum computing, FAIR data, technical training and the embedding of green computing in community workflows. Please link these with your formal workplans wherever sensible.

The reporting period started with a visit by Prof. Mark van Schilfgaarde who was invited to be CCP9 Distinguished Lecturer and gave 5 talks within a one-week tour of UK Universities, giving Invited Talks and Departmental Colloquia at St Andrews, Warwick, London's Thomas Young

Centre, Loughborough as well as at Rutherford Appleton Laboratory. Mark van Schilfgaarde is Chief Theorist at the USA's National Laboratory of the Rockies (formerly NREL) and is one of the leading experts globally on condensed matter theory. The visit took place 8-12 September 2025 (but was not reported previously) and CCP9 sponsored and arranged travel and accommodation for the tour.

Ongoing activity in support for Wannier90 resulted in a very successful programming and training event that took place at Imperial College London (25-27 March 2026) and included 25 developers representing the main DFT codes worldwide (quantum espresso, VASP, Wien2k, CASTEP, etc) who came together to adopt the new Wannier90 version.

Software developments in ONETEP and CRYSTAL were delivered focusing on effective GPU utilisation. In ONETEP, developments by Manuel dos Santos Dias have focused on adapting ONETEP's sparse memory machinery for effective host/device memory transfer. In CRYSTAL, Barry G Searle has improved energy efficiency allowing caching of specific intermediate results according to the different memory/compute availability on GPU machines relative to operation on CPUs alone. Developments in CRYSTAL were additionally supported by the eCSE project "GCRYSTAL – A GPU enabled CRYSTAL".

The reporting period featured initiation of a new collaboration between CCP9 members at the universities of Durham, Oxford, Birmingham, Manchester and STFC's Jerome Jackson (CCP9 Scientific Secretary/Project Lead) in developing a new software utility intended to automate the extraction of crystal field parameters for transition and f-block ions in different crystal environments: this is particularly valuable for modelling and interpreting many experiments including x-ray and neutron scattering processes, for example with battery materials applications.

CCP9 members and core support team were successful in obtaining Software Sustainability Institute grants to provide additional maintenance support for the key CCP9 codes CASTEP and Wannier90; this call which was open to all scientific and non-scientific disciplines in UK academia, attracted extraordinary interest and the award of two grants highlights the importance of CCP9 software even when viewed from the broadest perspective.

3. Research Implications and Impact

4. Up to 5 research outputs that create an impact story for your community

- CCP9 core support team member Manuel dos Santos Dias presented an invited talk on "Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3" at the JCNS Workshop 2025, Trends and Perspectives in Neutron Scattering. Quantum Materials: Theory and Experiments that took place on 7 – 9 October 2026 in Tutzing, Germany. He also chaired the session titled "Models of quantum magnetic systems". https://iffindico.fz-juelich.de/event/20/

- With his collaborators at Diamond Light Source and Charles University, Manuel dos Santos Dias also published the impactful paper "Systematic mapping of altermagnetic

magnons by resonant inelastic X-ray circular dichroism", Nat Commun 16, 9311 (2025), DOI: 10.1038/s41467-025-64322-0

- The Electronic Structure Library held a workshop Zaragoza, Spain, sponsored by CCP9, CCP-QC, CECAM and Psi-k https://esl.cecam.org/en/events/esl11/

5. Workshops and new opportunities*

- "Daresbury DFTB+ school", 15-19 June 2026, STFC Daresbury Laboratory, https://www.cecam.org/workshop-details/daresbury-dftb-school-1550
- "TYC 8th Energy Materials Workshop: From Electron and Phonon Interactions to Net Zero", 1-3 July 2026, King's College London, https://thomasyoungcentre.org/event/tyc-8th-energy-materials-workshop/
- "Tackling the Many-Body Problem in Condensed Matter with Quantum Computing", 1-3 July 2026, University of Strathclyde, https://ccp-qc.ac.uk/ws_mb/
- "Recent Appointees in Physical Chemistry 2026 RAPC-RSC2026", 7-9 September 2026, Birmingham, https://rapc-rsc2026.github.io/
- "GAP and (M/GR)ACE users and developers meeting", 7-10 September 2026, University of Warwick
- "Wannier90 Developer Meeting", 7-11 September 2026, Trieste, https://www.cecam.org/workshop-details/wannier90-developer-meeting-1541
- "MSSC2026 - Ab initio Modelling in Solid State Chemistry, London Edition", 14-18 September, Imperial College London, https://www.imperial.ac.uk/mssc/mssc2026/

6. Issues and problems*

Lack of clarity in the status of the EPSRC-network, EPSRC-core-support, DRI-network, DRI-core-support extension status has caused significant difficulty:

1. no provision for ongoing community network support (new events beyond lifetime of original grants),
2. challenges in organising EPSRC-core-support and DRI-core-support workplans as extensions have been extended,
3. general dissatisfaction was expressed among many of the community at a recent large community assembly because of lack of clarity in CCP renewal process, and
4. difficulty for the Chair/Secretary/team in coordinating the community to prepare for unknown renewal process.

Long term staff illness in the core support team at STFC has risks some underspend that remains difficult to address because of programme uncertainty and STFC recruitment chill.

Biological Science

CCP BioSim for the Period 01/10/25 to 31/03/26

Prof. Sarah Harris (CCP-BioSim Chair), Dr. James Gebbie-Rayet (CoSeC Project Lead)

1. Background

CCPBioSim, the Collaborative Computational Project in Biomolecular Simulation operates at the interface of physics and life sciences, uniting chemists, physicists, chemical engineers, and researchers across all disciplines of molecule-oriented biochemistry and biology. Computational simulation plays a central role in advancing our understanding of how enzymes catalyse biochemical reactions, how proteins adopt their functional structures within complex environments such as cell membranes, and how molecular mechanisms underpin disease. These capabilities directly inform the design of drugs and catalysts, bridging the gap between fundamental research and practical application. Central to our mission is the integration of experimental and computational approaches, founded on the conviction that the most impactful science emerges from the close collaboration of theorists and experimentalists.
CCPBioSim is equally committed to building a skilled and inclusive research community. Through a comprehensive programme of tutorials, workshops, and training initiatives, we support early career researchers and non-specialists in developing proficiency in biomolecular simulation techniques. We also drive the development of advanced methodologies that will underpin the next generation of scientific discoveries across our community. Our specialised industrial engagement seminars provide a forum for academic and industry researchers to exchange insights and showcase work that reflects the distinct priorities of applied research. In addition, CCPBioSim maintains a strategic partnership with the structural biology CCPs - CCP4, CCPEM, and CCPN through the DRIIMB initiative, a UKRI DRI-funded community project focused on integrative molecular biology and software interoperability.

2. Outputs

A significant priority for our community is the development of CodeEntropy https://doi.org/10.5281/zenodo.17570721, which is our flagship software for applications in drug discovery. In the report period there has been 10 releases. CodeEntropy has seen a broad range of improvements spanning new scientific features, bug fixes, and infrastructure modernisation. Key scientific additions include basic orientational entropy calculations, force halving for flexible dihedrals, trajectory slicing, force partitioning, LAMMPS compatibility, and support for entropy calculations where forces and coordinates are held in separate files. Numerical correctness was improved through fixes to transvibrational entropy, invalid eigenvalue handling, and alignment of entropy methods with the 2019 paper, alongside the adoption of principal axes for translational and rotational coordinates at all levels and a change

in light atom selection from name-based to mass-based criteria. Performance was enhanced through optimisation of the RAD neighbour search and blocking loop, and the workflow was refactored to a DAG architecture with deterministic group ordering across the pipeline. On the testing and CI side, a scenario-based regression testing framework was introduced, along with expanded configuration coverage, an automated baseline update workflow, and a separated MDAnalysis compatibility workflow with an expanded OS matrix. Distribution was improved through the addition of Conda packaging with automated Anaconda publishing, and Python 3.14 support was added. Dependency management was modernised via migration to the official Renovate GitHub App, PEP 621 support, and automated copyright updates, with documentation also updated to include regenerated API docs, standardised Google-style docstrings, and improved getting started guidance.

CCPBioSim has adopted two new software packages aiida-amber https://doi.org/10.5281/zenodo.18400803 and aiida-gromacs https://zenodo.org/records/18838601 and will co-develop these with initiatives in the PSDI data infrastructure programme. Work in this period has been to establish the CCPBioSim adoption process and modernise the CI and release framework and to bring the software tools in line with the community established best practices for long term software maintenance.

We have significantly modernised our digital training infrastructure in the cloud, work has significantly altered the way that these are built and maintained. We now have continuous deployment of training containerised images; multi-architecture builds and automated dependency management. This will enable us to scale our management and development of training courses to much larger numbers whilst eliminating the very resource intensive process of keeping them up to date with the rapidly evolving tools in the field. We have developed templates for new courses to be developed to assist researchers with creating new training materials.

The CCPBioSim Training week was 13-17 October 2025, with 26 students receiving training on the basics of biomolecular simulations and an introduction to machine learning for simulation analysis.

The Industry Talks series is one of our biggest successes. The talks are always interesting with topics including computational science, experimental work, and careers. They are well attended with audiences between 50 and 150 people. They give opportunities for connections between industry researchers and the academic members of our community. The following list was ran:

- DRIIMB seminar on BioSimDR — 7 November 2025
- CCPBioSim Industry Talk – Ted Smith — 5 November 2025
- Industry Talk – Sygnature Discovery — 14 January 2026
- DRIIMB webinar by Helen Berman: Building Community Data Resources for Structural Biology — 27 January 2026
- Industry Talk – Schrödinger — 11 February 2026
- DRIIMB webinar: Current state of data standards, repositories, and interpretation approaches for structural modelling with mass spectrometry data — 24 February 2026

- DRIIMB webinar: AI in the biosciences (AIBIO-UK) — 3 March 2026
- Industry Talk – ChemCompGroup — 11 March 2026
- Industry Talk – Boehringer Ingelheim — 22 April 2026
- DRIIMB webinar: Solving 3D puzzles of biomolecular interactions by physics- and AI-based integrative modelling by Prof. Bonvin — 29 April 2026

3. Research Implications and Impact

The developments in this period of our flagship CodeEntropy have brought this new methodology toward a state of real-world readiness. Entropy is conceptually difficult and impossible to quantify directly using experimental methodologies, however understanding it is vital in the pharmaceutical industry for the discovery of new drugs. This method is very new and is now starting to generate significant interest from researchers and industry in its application to drug-binding prediction workflows. This code represents the most complete implementation of entropy theory and likely the first production grade tool for the application to this type of problem. It directly competes with Free Energy based methods where CodeEntropy is 10 times more computationally efficient whilst also quantifying information of direct application to drug discovery.

The data tools whilst also very new, are expected to enable our community to change the way we produce, curate, store and share data. Whilst the infrastructure behind BioSimDB is developed by PSDI, these software tools are designed to bring about culture change without the pain of having to adopt totally new ways of working. They will enable researchers to seamlessly capture full data provenance and automatically annotate their workflows against emerging data standards at the EU level, enabling fully transparent, full reproducible (FAIR) and standardisation of the ways we publish, share and reuse our research.

4. Up to 5 research outputs that create an impact story for your community

CodeEntropy is a good story because it is a scientifically important code that is emerging, but it also highlights the strengths of having a programme like CoSeC to underpin the communities. The lead academic that was developing the theory has left the UK and retrained as a medical doctor. Without CoSeC and CCPBioSim this vitally important new method with huge industrial potential would have disappeared completely. The strength of the community backed by software developers at STFC have enabled this code to be realised and will now start to be exploited by researchers and industrialists around the world.

5. Workshops and new opportunities*

- Monthly Online Industry Talks – planned until March 2027, the next one is 27 May 2026 (wider interest for other communities)
- Integrated Modelling and Scattering for Biomolecules – in Sheffield, 18 – 20 May 2026, www.ccpbiosim.ac.uk/scattering2026
- Multiscale Biomolecular Simulations with ChemShell – training workshop at Daresbury Lab, 4 June 2016, www.ccpbiosim.ac.uk/chemshell2026
- Annual Conference – in Bristol, 6-8 July 2026, www.ccpbiosim.ac.uk/bristol2026

- DRIIMB Conference and Software Skills Workshop – in Leeds, 12 – 16 October 2026
- CCPBioSim Training Week – in Sheffield, 28 September – 2 October 2026, www.ccpbiosim.ac.uk/training2026
- CodeEntropy Users Group Meeting, details to be determined

6. Issues and problems*

The main issue facing our community as well as other communities is that of funding. The uncertainties around whether these vital programmes of work will continue into the future, which parts and funded by which councils make community planning very difficult.

CCP4 for the Period 01/11/25 to 29/05/26

Prof. Ivo Tews (CCP4 Chair)

1. Background

CCP4 provides and supports an integrated suite of programs for determination of macromolecular structures by X-ray crystallography. CCP4

- develops cutting edge approaches to experimental determination and analysis of macromolecular structures as a community-based resource;
- supports the development and integration of novel software into one suite;
- serves the widest possible research community, embracing academic (not for profit) and industrial (for-profit) research;
- offers education and training to scientists in experimental structural biology and encourages the wide dissemination of new ideas, techniques, and practice.

2. Outputs

CCP4 was asked to present at two **national events**:

- Inaugural CCP-volumeEM Community Meeting “Towards a collaborative computational community for volume EM”, London, Francis Crick Institute, 3.11.2025
- Instruct/ERIC UK Structural Biology Roadmap Town Hall: Discussion of community needs and priorities for the Next Decade, London, Wellcome Collection, 12.5.2026

We have run several **conferences and workshops**, as listed in section 5. For more information see:

- https://www.ccp4.ac.uk/workshops/

The BBSRC funded **CCP4 research grant** that started 08/24 includes four work packages that have created individual output, leading to reported publications (Research Fish), and presented at national and international conferences:

- **WP1** A statistical framework for analysing structural change and its representation in data (time and/or state); Diamond Light Source; PDRA started 10/24.
- **WP2** Joint refinement of related structures; LMB Cambridge; University of Southampton, University of York; PDRA started 11/24.

- **WP3** Advance computational methods for data processing and structure solution to exploit advantages in electron diffraction; Research Complex at Harwell; PDRA started 07/25.
- **WP4** Exploiting Deep Learning-based structural bioinformatics for crystallography; University of Liverpool; PDRA started 09/24.

The **grant team report** to the community at the annual CCP4 study weekend (January each year) and at the CCP4 Developers meeting and to the CCP4 executive (both July each year).

The **Core Group** have rolled out six updates since November 2025. For details see here: https://www.ccp4.ac.uk/ccp4-9-0-updates/:
- Update v.9.0.12, 12.12.25
- Update v.9.0.13, 20.01.26
- Update v.9.0.14, 20.02.26
- Update v.9.0.15, 16.04.26

The **CORE GROUP report** at the CCP4 Developers meeting (July each year), at the annual CCP4 study weekend to the user community, and to the CCP4 executive (quarter annually).

The **CCP4 Equity, diversity & inclusion team** have developed a roadmap to equal and diverse participation for CCP4, see https://www.ccp4.ac.uk/ccp4-equity-diversity-inclusion/.

The **CoSeC funded "Digital Research Infrastructure for Integrative Molecular Biology (DRIIMB)"** (since 11/24) meets monthly as a consortium of CCP4 (who presently chair) with CCPEM, CCPBioSim and CCPN. CCP4 has two work packages each with an associated. See also separate report. Visible outputs are the successful ISMB meeting in Sheffield and the planned ISMB meeting in Leeds, 10/26.

Activity in **obtaining additional funding** is successful. Thera are presently several posts funded through grants and organisations which are associated with CCP4. These include DRI, CoSeC, ALC, BBR24, BBSRC and BBSRC/NSF.

3. Research Implications and impact

The field are looking intensely on development of the computing suite, for example in working group 2 meetings. CCP4 is migrating from use of GenAI structural models to specifically enhance computing with implementation of AI methodology and user experience. Novel software solutions have already been explored and shared between programmers at the CCP4 retreat (03/26). These discussions will continue with the wider Developers community at the CCP4 review meeting (07/26).

4. Up to 5 research outputs that create an impact story for your community

Since it was published, the primary publication for CCP4 (Acta Crystallogr D Struct Biol. 2023, 79:449-461. doi: 10.1107/S2059798323003595) has been cited more than 600 times, with more than 4.5k downloads in PDF format and 18.7+ k HTML views. There are many high impact publications on scientific application of the software, including in Nature-, Science- and Cell-

group journals. Citations also accumulate in the field of AI use, in particular with respect of the use of AlphaFold in structural biology.

5. Workshops and new opportunities*

See here: https://www.ccp4.ac.uk/workshops/

The CCP4 study weekend held in January each year is a highlight event and of interest for other communities; attendance gives opportunity for cross community (net-)working, but online participation is also possible. The meeting gives a good overview on current trends.

List of main meetings organised or supported by the CCP
2025

- CCP4/DLS Data Collection and Structure Solution Workshop, November
- CCP4 Northern Structural Biology Meeting, November
- AsCA, Taipei, December

2026

- CCP4 Study Weekend, January
- CCP4 Central European Workshop, May
- CCP4 Developers meeting, July
- CCP4 SWSBC Cardiff, July
- CCP4/APS School in Macromolecular Crystallography, July
- CCP4 - BCA Summer School, Jon Innes Centre September
- CCP4 Northern Meeting November

6. Issues and problems*

Technical issues of rolling out the suite to users are being addressed with a change in the distribution model. The issues were discussed at the CCP4 retreat (03/26), and a proposal will be discussed with the developers' community at the CCP4 review meeting (07/26).

- We are faced with an ever-growing number of dependencies in the software suite; we presently require 600+ packages and 400+ patches to release the software bundle. We are testing UV and Micromamba, as well as on-demand downloadable extensions.
- OS evolution provides a further challenge, as we provide software for three platforms leading to incompatibilities in some of the software packages; migration to newer frameworks are costly developments, given the complexity of the suite.
- Efficient use of heterogeneous compute architecture is a goal, along with efficiency improvements for better using resources. We are specifically looking at novel GPU solutions for standard compute-intense crystallographic problems (e.g. ligand identification/fitting).
- We must provide for heavy LLM and CNN libraries, which will extend the size of the distribution; hence a server architecture for these applications is envisaged.
- With these developments, we must provide solutions that cater for the entire user community, to be inclusive to users with less powerful compute equipment; this provides a major challenge.

We would like to note that **contract issues are continuing to impact this network**. These concern mainly the length of negotiations required to finalise paperwork. We would like to see

that decisions taken be the CCP4 executive are speedily realised to avoid a wasteful process (human resource for contract negotiations; loss of funds by moving conclusion of contracts into subsequent financial years).

In their roadmap, the **CCP4 Equity, diversity & inclusion team** propose mechanisms to provide for equal and diverse participation, and for fairness and equitable access to collaboration and funding. These proposals are being discussed and require implementation, which will also mean that mechanism must be created to measure the impact of changes made.

CCP-EM for the Period 01/11/25 to 01/05/26

Tom Burnley (PI and Project Lead), Prof Maya Topf (CCP-EM Chair)

1. Background

CCP-EM brings together a diverse and rapidly growing community of researchers involved in cryogenic electron microscopy. The project develops and supports a software suite for structure determination by single particle analysis and subtomogram averaging, including the interpretation of cryoEM maps in terms of atomic models. The suite includes contributions from many collaborating groups in the UK and internationally.

A recent major development has been the implementation of the *ccpem-pipeliner*, which supports workflow metadata management, archiving, and deposition to public repositories including EMPIAR, EMDB and the PDB. The *Doppio* user interface builds on this framework, providing a modern JavaScript-based interface that enables web-based operation and remote submission of compute jobs.

CCP-EM also organises and supports a wide range of training activities. Its annual Spring Symposium now attracts more than 350 in-person delegates and provides an important forum for the cryoEM community.

Machine learning techniques are already embedded across the current software suite and are central to future plans, including applications such as object recognition, classification and denoising.

2. Highlights for the current reporting period

Funding: MRC Partnership grant started “Collaborative Computational Project for cryo electron microscopy (CCP-EM): expanding the reach of cryoEM”. This provides core funding and provides ~3FTEs and spans 01/03/2026 to 28/02/2031. Cols: Martyn Winn (STFC), Giulia Zanetti (Birkbeck, University of London, CCP-EM Co-chair), Peijun Zhang (Diamond Light Source), Kyle Morris (EMBL), Maya Topf (Leibniz Institute of Virology, CCP-EM Chair), Sjors Scheres (MRC Laboratory of Molecular Biology), Peter Rosenthal (The Francis Crick Institute), Paula da Fonseca (University of Glasgow).
Grant started on time, all posts filled.

Software: Version 1.5.0

2nd February 2026

Doppio updates

- Allow each Doppio server instance to work in a different project
- Include category names when searching for new jobs
- Add tooltip messages to explain why deactivated job options have been deactivated
- Fix bug that caused Plotly plots to reset their state occasionally
- Add SSL options to allow Doppio to be used with HTTPS
- Switch to Python 3.10

Job updates

- Fix issue passing correct Topaz executable name to both RELION 4 and 5
- Improve results display for Aligned Average Power Spectrum job
- Add ability to continue a MotionCorr job to regenerate output micrographs from previously-calculated shifts
- Add option to calculate helical particle positions by specifying box overlap fraction
- Rename some jobs for consistency: “em_placement” is now “EMPlacement” and EMDA jobs include “EMDA” in their names
- Various minor bug fixes and updates

Pipeliner updates

- Update Python version range to include 3.12, 3.13 and 3.14
- Update to use latest versions of Gemmi, NumPy, SciPy and Pillow
- Various minor bug fixes and updates

Software: Version 1.6.0 beta

17th April 2026

Doppio updates

- Major update of Moorhen integration for increased workflow flexibility and improved file handling
- Add ability to edit and save picked particle coordinates
- Add support for displaying RELION’s angular distribution .bild files in the Mol* viewer
- Make Doppio installer more self-contained by including more required libraries
- Add additional package definition for LTM template matching software
- Update to Material UI v7
- Various minor bug fixes and improvements

New jobs

- Add job for joining tomogram and tilt series STAR files
- Add jobs for mask creation and template matching using LTM software

Job updates

- Add angular distribution plots and 3D .bild file display to Refine3D job results
- Expand and improve results display for MetalCoord, Servalcat Refine and CryoEF jobs
- Add ability to use custom atomic form factors in Servalcat Refine job
- Standardise job options for all helical refinement jobs
- Improve handling of imported particle coordinates in .box format
- Add tomography node types to the Import job
- Various minor bug fixes and updates

Pipeliner updates

- Update job options to use correct internal value types
- Various minor bug fixes and updates

Annual Conference: 12th CCP-EM Spring Symposium 22-24 April 2026
The 12th CCP-EM Spring Symposium incorporated the Diamond Biological Cryo-Imaging (BCI) User Meeting and the Karen Davies Memorial session.

The meeting was attended by 312 in-person delegates, who travelled from 16 countries across four continents. Of these, 81% were from the UK, 14% from Europe (ex. UK), with additional delegates from North America, Asia and South America. The online programme attracted 635 unique virtual delegates, with a mean viewing time of four hours.

A total of 100 posters were presented, primarily by early-career researchers. More than £30k of commercial sponsorship from nine companies enabled 35 bursaries for in-person attendance. The scientific programme featured world-leading talks on method development and exemplar applications, with speakers from institutes including EMBL-EBI, MRC-LMB, the Rosalind Franklin Institute, the Max Planck Institute of Biophysics, Human Technopole, and the Universities of Leeds, Leicester, Oxford, Columbia and Washington State.

Workshops

- **9th Icknield Model Building Workshop**, Harwell Campus, 13–17 October 2025. This five-day course was aimed primarily at structural biologists with EM maps suitable for model building and refinement.

- **Doppio Roadshows**, University of Manchester, November 2025, and Dundee/St Andrews, March 2026. These one-day workshops introduced researchers to SPA and model building workflows in Doppio.

- **Model Building and Validation Workshop**, National Centre for Biological Sciences, Bangalore, India, 30 March – 3 April 2026. This five-day workshop covered different stages of the model building workflow.

Training courses are usually run using the STFC Ada training system, previously known as DAaaS, running on STFC Cloud VMs with or without GPU support, with Doppio and example data pre-installed. User access is managed through the DAaaS training website and proxy. The Doppio app runs in the user's local browser, providing a faster response than a remote desktop. We have also collaborated with Dectris to set up our software stack on their commercial cloud platform for workshops when the STFC Cloud is not available, for example during maintenance periods.

3. Overview of work relating to accelerated computing

There is an urgent need to accelerate RELION, which is widely used for single particle reconstruction and subtomogram averaging. These are computationally demanding workflows, processing gigabytes to terabytes of image data per dataset. RELION is used in many laboratories worldwide, forms part of the automated processing pipeline at eBIC and is associated with more than 14,000 public depositions in the EMBL-EBI Electron Microscopy Data Bank (EMDB). It is a critical component of the Doppio software suite, but is under pressure from

commercial competitors, particularly because of the faster speed of some competing workflows.

Working with the lead developer, Sjors Scheres at MRC-LMB, and the OxRSE group, we extensively profiled the code to identify key processing bottlenecks. These were found in 2D and 3D classification and 3D reconstruction, particularly in the expectation calculation. These routines were ported to GPUs around 10 years ago and now require re-optimisation for modern hardware.

Through ALC funding, we are currently optimising these routines and have achieved a 3–4× speed-up in the expectation step, depending on the dataset and hardware used. This work is ongoing, and we aim to exceed a 5× speed-up before completion in July 2026.

4. Current plans, developments, or specific applications of AI

AI and machine learning techniques are now in widespread use for interpreting large cryoEM datasets. Several ongoing AI/ML projects are underway, including: (1) affinity-VAE, for automatic clustering and classification of objects in cryoET tomograms, in collaboration with the Rosalind Franklin Institute; (2) cryoDANN, using domain-adversarial training of neural networks for particle selection as a refinement of the 2D classification step for particle-set cleaning; (3) a Noise2Noise implementation for denoising tomograms; and (4) support in Doppio for AI/ML-based heterogeneous reconstruction algorithms, including DynaMight, cryoDRGN and RECOVAR.

Through the DRI-IMB project, and in collaboration with Princeton and the Flatiron Institute, we launched the Community-Wide Assessment of CryoEM Heterogeneous Reconstruction Algorithms (CAHRA). This project is developing three datasets with testable ground truth to objectively quantify the performance of next-generation AI/ML-based reconstruction tools currently being developed in the cryoEM community. The challenge and datasets were launched in November 2025 through a webinar attended by more than 60 researchers. Entries for the challenge close in June 2026, and a review workshop will take place at RAL in September 2026.

5. Up to 5 research outputs that create an impact story for your community from the reporting period.

2026

- CoSeC Software Spotlight: CCP-EM Doppio: https://www.cosec.ac.uk/impact/software-spotlight-may-2026/

2025

- Automated filtering of particle images in single particle cryoEM. S Malhotra et al, BioRxiv, https://doi.org/10.1101/2025.11.12.688030
- Ten years of the CCP-EM Spring Symposium. L Giles, T Burnley. Biological Crystallography 81 (12), 656-659

- PERC: a suite of software tools for the curation of cryoEM data with application to simulation, modeling and machine learning B Costa-Gomes, et al., Structural Biology and Crystallization Communications 81 (10)
- Engineering Supercomputing Platforms for Biomolecular Applications R Welch, et al. arXiv preprint arXiv:2506.15585

6. Workshops and new opportunities*

- Erice International School Crystallography, Italy, May 2026
- Dutch cryoEM school, Leiden/Delft, Netherlands, June 2026
- MSCDA cryoEM course, Exeter, Sep 2026
- CAHRA Heterogeneity challenge, Sep 2026
- China National Facility for Protein Science, Sep 2026
- Icknield workshop, RAL, Nov 2026
- King Mongkut's, Thailand, Nov 2026
- 13th CCP-EM Spring Symposium and DLS BCI User Meeting, East Midlands Conference Centre, Nottingham University, April 2027

7. Issues and problems*

Note concern and willingness to support efforts to secure long-term funding for CoSeC.

DRIIMB for the Period 01/10/25 to 31/03/26

Sarah Harris, Chair CCPBioSim

1. Background

The Digital Research Infrastructure for Integrated Molecular Biology (DRIIMB) project is a collaborative initiative involving multiple Collaborative Computational Projects (CCPs), including CCPBioSim, CCPN, CCP-EM and CCP4. The project aims to develop interoperable digital research infrastructure and computational workflows that support integrative structural biology and biomolecular simulation.

CCPN - CCPBioSim

This work package (WP) focuses on improving the accessibility and reproducibility of molecular dynamics simulations for the biomolecular NMR community. This involves developing workflows that connect experimental NMR data handling in CCPN with biomolecular simulation approaches used within CCPBioSim. The aim is to enable researchers to move more easily from NMR data analysis to MD simulation, structural interpretation and ensemble analysis, while reducing dependence on command-line tools and improving access to reproducible, HPC-enabled workflows.

CCPBioSim

The aim of this work package is to develop tools to allow files from the Protein Data Bank (PDB) to be used in molecular dynamics (MD) simulations. The contents of these files are subject to the physical limitations of experimental imaging methods; there are missing residues, missing

atoms, heteroatoms and steric clashes. Fixing these problems is currently a labour-intensive, manual process. However, the Python ecosystem for computational biology has recently become mature enough that many of these problems can be solved though python packages with well-defined APIs, enabling the creation of an automated system preparation pipeline.

CCP-EM

The conformational and compositional heterogeneity of biological macromolecules leads to the functional processes which occur in all living organisms. Through electron cryo-microscopy (cryo-EM) imaging, discrete conformational and/or compositional states of these macromolecules in a purified or in-situ (cellular) environment can be recovered. Over the last 10 years heterogeneous reconstruction algorithms (HRAs) to interpret and represent the full range of heterogeneity present in cryo-EM datasets have been developed. However, their performance in faithfully recovering different types of heterogeneity is still poorly understood. To address this, we are running the "Community-wide Assessment of cryo-EM Heterogeneous Reconstruction Algorithms" (CAHRA) Challenge to drive benchmarking of HRAs on (large) datasets with known ground truth information. This utilises an integrative approach, such as the use of MD simulation (and collaboration with CCPBioSim) for generation of synthetic cryo-EM benchmark datasets and allows for the exploration and benchmarking of HRAs, whether or not a particular HRA uses an integrative approach or not. The CAHRA challenge acts as a community hub for heterogeneity analysis on cryo-EM datasets, and is driving development and utilisation of HRAs, as well as of both benchmarking datasets and benchmarking metrics. Other work includes extending our understanding of how heterogeneity derived through other techniques such as NMR and MX fit in the conformational space explored through utilisation of HRAs on cryo-EM datasets (and their exploration of extremely long timescales compared to NMR). Through this we can explore how HRAs can optimally be used in integrative approaches to understanding structural biology.

CCP4

CCP4 has two work packages associated with DRIIMB. We probe heterogeneous computing with the CoSeC STFC post Dr Daniel Celis Garza (concluded) and investigate data structures data integration across different experimental techniques, funded post Dr Toby King (running).

2. Outputs

Hima Bindu Kolli - CCPN – CCPBioSim

A major output during this period has been the continued development of a GUI-based NMR-restrained molecular dynamics (NMR-MD) workflow integrated directly into CCPNmr AnalysisAssign on NMRbox. This includes both simulation setup and execution, as well as dedicated analysis and visualisation modules to support interpretation of MD trajectories by experimental NMR users. Substantial effort has been dedicated to integrating HPC capabilities into the workflow through HTCondor support on NMRbox, enabling users to run simulations locally or on HPC resources while maintaining organised, reproducible workflow outputs.

- Development of an integrated NMR–MD workflow with analysis and visualisation modules within CCPNmr AnalysisAssign

- HPC and reproducible workflows
- Community engagement and training activities
-

Activities across DRIIMB and related CCP communities included supporting the organisation of the DRIIMB webinar series, preparing technical demonstrations and user workflows, contributing to conference abstracts and dissemination materials, and developing training documentation and setup instructions for users.

Rob Welch – CCPBioSim
The output of this WP is prepmd, a python package that can automatically download structure and sequence data from the PDB and other repositories, fill in missing residues, fix missing atoms and non-standard residues, remove or extract and fix heteroatoms\ligands, and resolve steric clashes. Prepmd can reliably produce ready-to-use structure files from PDB entries that contain large missing regions, ligands and which have extremely high clash scores. As part of the system preparation process, it automatically validates that output structures are suitable for MD runs, and can also run production MD simulations for testing, validation, visualisation and minimisation. prepmd can automatically select MD parameters such as the numerical integration scheme and nonbonded interaction method for optimal performance and accuracy.

This pipeline connects many disparate python packages from the computational biology ecosystem, including MODELLER, pdbfixer, rdkit, OpenMM and MDAnalysis, automatically ensuring that each tool has the data and file format it requires. Although the pipeline is automated, it's not a 'black box', providing users with a lot of options, outputting detailed information about the changes being made to the structure, and warning about possible issues in structure files and inputs.

In addition to being available as a standalone python package, we are currently working on adding prepmd to existing computational biophysics software bundles, such as NMRBox and the CCP-EM software suite, and making it accessible through interfaces such as CCP-EM Doppio.

Joel Greer – CCP-EM
I have established and manage a collaboration with Ellen Zhong (Princeton University), Pilar Cossio and Sonya Hanson (both Flatiron Institute), all of whom are leading experts in the extraction of heterogeneity from cryo-EM datasets to create the CAHRA Challenge. We launched this in Nov 2025, including a launch webinar. More details (including the webinar) can be found on the CAHRA Challenge website (https://heterogeneity.notion.site/challenge). We received preliminary entries to the challenge in March. I have written a software suite of tools to automate the calculation of metrics on these datasets which will be published after the Challenge review meeting in Sept. I have also been extending and maintaining the roodmus software suite which is utilised to create challenge dataset (https://github.com/ccpem/roodmus) and ran pilot studies for validation and verification of the challenge datasets before release.

Daniel Garza – CCP4

The pilot project in heterogeneous computing started with looking at the Molecular Replacement problem, a central computing task in macromolecular crystallography. However, this problem turned out to be unsuitable for GPU-based parallelisation due to the special way in which the FFT contributions have to be summed. Attention turned to a different problem, the fitting of ligands into electron density maps. While small gains can be achieved for original code (1.2-2x), complete re-design of the code base to reach 6x to 8x performance improvement in the GPU-parallelisable section. While this exercise was useful, future directions will be to enable parallel crystal screening by wrapping into a parallel process.

3. Research Implications and Impact

Hima Bindu Kolli - CCPN - CCPBioSim
The integration of NMR data handling, molecular simulation, and trajectory analysis within a unified graphical environment has the potential to significantly reduce technical barriers for experimental researchers adopting computational approaches. The integration of automated workflows and reproducible analysis pipelines is expected to improve uptake of biomolecular simulation methodologies among non-expert users while facilitating more robust and transparent computational research practices.

Rob Welch – CCPBioSim
prepmd has already been publicly released on CCPBioSim's GitHub page and can also be installed via the CCPBioSim conda channel, with work to integrate it into other CCP software packages currently ongoing. This will enable much faster and easier preparation of MD simulations for novice and experienced MD users, could allow for the creation of large ensembles of simulations without the need for manual preparation, and allows for the construction of larger, multi-step structure refinement pipelines to improve the quality of structural data. We are currently exploring collaborations that would enable an automated pipeline for ensemble reweighting, which would allow for better characterisation of MD structural ensembles and quantification of errors in EM data.

Overall, this project has resulted in closer and easier coupling between EM and MD software and workflows, and it enables a two-way collaboration between both fields – MD modellers can use EM structures more easily, and EM users can make use of MD to perform validations and structural refinements.

Joel Greer – CCP-EM
Utilisation of HRAs to better understand conformational and compositional changes in protein structure has wide-reaching potential, including in the development of drugs or study of plant resilience to climate change. In the closer term, the expected performance of these algorithms on certain types of heterogeneity in poorly understood. Through benchmarking on CAHRA challenge datasets the cryo-EM community can both develop/improve approaches and understand where limitations lie. It also highlights the most successful approaches. As HRAs are often complex to use, install and analyse the outputs of, this allows for identification and prioritisation of techniques and software to integrate with user-friendly GUI-based software pipelines. For example, CryoDRGN has been integrated into CCP-EM's Doppio software suite. The community would benefit from the most valuable other programs also being made

available. Whilst CAHRA utilises single-particle-analysis datasets, this is a first step, with future challenges having the potential to extend to in-situ tomography datasets. Whilst the challenge has a start and end date, the datasets provided to the community, as well as the submitted entries (once this challenge ends) will form a publicly available dataset facilitating further HRA and metric development. Exploration and interpretation of the heterogeneity present in cryo-EM datasets remains at the cutting edge of the field, facilitating both dataset analysis and exploration of the processes via which proteins function. Benchmarking this, in addition to exploration of integration with data from perpendicular approaches, such as NMR or MX are a high priority in the field.

Toby King – CCP4
The scoping exercise to determine whether additional value/ information can be gained by the inclusion/processing of multiple data types/sources in a single model delivers code integrated into the Moorhen visualisation package. The first successful experiments are parsing of NEF data formats coming from NMR as well as Map formats coming from Small Angle Xray Scattering analysis. Reading and working with EM data as well as parsing to biomolecular simulations are tasks that will be explored in this project in future.

4. Up to 5 research outputs that create an impact story for your community

Hima Bindu Kolli - CCPN - CCPBioSim
The NMR-MD workflow provides an end-to-end graphical interface that enables experimental NMR users to prepare, run, monitor and analyse biomolecular simulations directly from NMR-derived structures and restraint data.

This output strengthens the connection between CCPN and CCPBioSim by linking experimental NMR data handling with reproducible biomolecular simulation workflows. It supports system preparation, restraint handling, AMBER-based simulation setup, local and HPC execution, trajectory analysis and visualisation within a single accessible environment. Its impact lies in lowering the technical barrier for NMR researchers to use MD simulations, while promoting reproducible, FAIR and interoperable workflows across the DRIIMB communities.

Rob Welch – CCPBioSim
The source code for prepmd has already released on the CCPBioSim GitHub, and a python package is available to download through CCPBioSim's conda channel. The research impact discussed in section 3 depends on user adoption, so we have developed an aggressive strategy for disseminating prepmd it within the community, through integration into existing software bundles and tools (such as the CCP-EM suite, pipeliner and CCP-EM Doppio), extensive user testing (both currently ongoing), workshops (planned for summer 2026) and talks ('prepmd: a truly automated system preparation pipeline for molecular dynamics simulations' submitted for the CCPBioSim 2026 conference) with a software publication to follow.

Joel Greer – CCP-EM

- Updates and additions to the roodmus software suite (available on CCP-EM's GitHub page) have been made to facilitate creation and publication of CAHRA Challenge conf-het dataset.

- The CAHRA Challenge has been released and is currently open (until June 1). In addition to community communication via the CAHRA Challenge, CCPEM and 3dem mailing lists, I presented at the launch webinar on 14th Nov (~70 attendees), and a talk at the CCP-EM symposium (April 2026) (~300 in person and ~300 online attendees).
- The CAHRA Challenge datasets have been created, validated and released for use in the Challenge
- I have written the software suite to calculate metrics on entries to the CAHRA Challenge – and this has been used to score the preliminary entries.
- Set up GPU CI for ccpem-pipeliner software (facilitating full testing of HRA (and other) plugins integrated in the Doppio software suite

5. Workshops and new opportunities*

Planned activities and workshops

- DRIIMB Conference and Software Carpentry Workshop from 12 - 16 October 2026 at the University of Leeds
- DRIIMB Webinar Series ongoing webinar series supporting cross-community engagement across CCPBioSim, CCPN, CCP-EM and CCP4.
- Integrated Modelling and Scattering for Biomolecules (IMSB) Meeting – May 2026 : meeting focused on integrative modelling, scattering approaches and biomolecular simulation, with relevance to multiple CCP communities.
- Planned summer workshops and training sessions for the NMR–MD workflow — training activities focused on introducing users to the NMR–MD workflow, including simulation setup, analysis, visualisation and reproducible use within CCPN/CCPBioSim workflows.
- CCPBioSim Conference 2026 — community conference supporting dissemination of DRIIMB-related work, including biomolecular simulation, interoperable workflows and links with experimental structural biology communities.
- **Planned summer workshops user testing for prepmd —** activities focused on testing and disseminating the automated MD system-preparation pipeline, with feedback sought from EM, crystallography and non-specialist MD users.
- **CAHRA Challenge Review Workshop** — September 2026 (https://heterogeneity.notion.site/workshop)
- **Cross-community data standards and interoperability activities** — opportunities to support integration of simulation and experimental data standards across CCPBioSim, CCPN, CCP-EM and CCP4.
- **Cross-CCP workflow collaboration** — continued collaboration between CCPBioSim, CCPN, CCP-EM and CCP4 on interoperable, reproducible workflows connecting NMR, MD, cryo-EM, crystallography and related structural biology approaches.

Overall, the work across the CCPs is helping to build FAIR, interoperable and user-friendly workflows that allow researchers to combine experimental data and simulations more effectively.

6. Issues and problems*

- **Software sustainability and maintenance:** As the NMR–MD workflow, prepmd and cryo-EM tools move towards wider use, sustained effort will be needed for long-term maintenance, compatibility updates, testing across different environments and user support.

- Some of the APIs used in prepmd are subject to change, which would require the software to be continuously updated, or it would eventually fall out of support and compatibility. New features, such as better file format support, new force field and new simulation options mean prepmd would benefit from active support and development over a period of years. prepmd makes use of several bleeding-edge methods, including the metadynamics features of openmm tools and small molecule force fields generated by openff. These features are not nearly as mature as those found in older MD software and will require thorough testing and validation. The need for a valid MODELLER license means that not all users can take advantage of all prepmd's features.

- **Usability and accessibility:** Speed and user-friendliness of using cryo-em processing software and pipelines. Doppio addresses the latter and Joel Greer will be supporting this through extending the testing architecture and writing tutorial documentation on how to utilise HRAs and analyse their outputs in this GUI.

Computational Engineering

CCP-WSI for the Period 01/10/25 to 31/03/26

Prof. Deborah Greaves (CCP-WSI Chair)

1. Background

The CCP in Wave Structure Interaction (WSI) began in October 2015 and was extended in October 2020 through the successful CCP-WSI+ proposal and then again through the CoSeC Bridging Fund to March 2027. The aim is to bring together and expand the national community of academics and industrial partners, working collaboratively on activities with a shared objective of building a Numerical Wave Tank (NWT) facility for the simulation of free-surface flow phenomena and fluid-wave interactions with complex structures. A range of networking activities, including focus groups, workshops, and road-mapping exercises, will provide a framework for innovation and the development of strategic software. The goal is to develop a robust and efficient computational WSI modelling tool capable of reliably quantifying wave-induced loads and the corresponding structural mechanics to supplement laboratory and field measurements early in the design process of associated structures. Throughout the project, with the assistance of CoSeC support (2.0 FTE), numerical modelers and experimentalists will combine their expertise to develop an open-source framework using state-of-the-art code coupling and parallelization practices. This enables the inclusion of highly nonlinear and multi-physics effects in simulations while reducing the overall computational effort required. The software, held in a central code repository, is professionally engineered, maintainable, and future-proof. It is also be tested and validated against measurement data from new fundamental benchmarking experiments. The project provides advanced training in

computational science and software development, as well as deliver outreach activities for schools and the general public.

2. Outputs

During this reporting period, CCP-WSI and HEC-WSI delivered significant outputs linked to the formal workplans on scalable WSI modelling, accelerated computing, benchmark development and multiphysics coupling. HEC-WSI activities focused particularly on GPU-enabled OpenFOAM development and performance-portable CFD workflows, supporting the transition of community WSI tools towards modern heterogeneous HPC platforms. CCP-WSI outputs focused on sloshing benchmark development and community validation, including dissemination through ISOPE 2025 and the continued development of the CCP-WSI Blind Test Series. Further progress was also made in scalable multiphysics coupling infrastructure through work on the Multiscale Universal Interface, supporting future coupled CFD, structural and multiphysics workflows. Technical capability building was supported through GPU-focused training activity, contributing to community upskilling in accelerated computing.

Significant outputs include:

- Presentations:
  - Wendi Liu, Merida, Yucatan, Mexico, Porting OpenFOAM on GPU via modern C++, ParCFD'2026, 37th International Conference on Parallel Computational Fluid Dynamics, 24–26 November 2025.
  - Yiyun Tan (Raynold), Cross-platform Programming Model for GPU Implementation of OpenFOAM Using ISO C++, ARCHER2 Celebration of Science 2026, 19–20 March 2026, Edinburgh.

- Papers:
  - Mayank Kumar, Jony Castagna, Mattijs Janssens, Raynold Tan, Wendi Liu and Gavin Tabor, Porting OpenFOAM on GPU via modern C++, ParCFD'2026 proceedings.
  - Scott Andrew Brown et al., A blind comparative study on isothermal sloshing in a circular tank (CCP-WSI Blind Test Series 5), *Ocean Engineering*.(under review)
  - Wendi Liu, Omar Ahmed Mahfoze, Mayank Kumar, Stephen M. Longshaw, Eduardo Ramos Fernandez and David R. Emerson, Multiscale Universal Interface v2.0: Lowering Barriers to Scalable Multiphysics Coupling, *Computer Physics Communications*.(under review)
  - Stella, J., Thompson, E., Margetts, L., & Papamarkou, T. (2026). "How transparent is water? Addressing ethical concerns in AI surrogate development for nearshore wave modelling and the natural sciences." *Journal of Ethics in Entrepreneurship and Technology*. https://doi.org/10.1108/JEET-06-2025-0043
  - Li, J., Sidebottom, M., Nabawy, M., & Margetts, L. (2026). "The aerodynamic outsiders: Life at the edge of flight", NAFEMS UK Conference 2026, Coventry, United Kingdom.

- Training:

- AMD Hackathon — Jony Castagna, Mayank Kumar and Tan Yiyun (Raynold), 3 participants × 3 days = 9 training days. HEC-WSI

3. Research Implications and Impact

Benchmarking and validation impact
The outputs described in Section 2 have supported the wider WSI community by improving confidence, reproducibility and best practice in numerical modelling of complex wave–structure interaction problems. In particular, CCP-WSI Blind Test Series 5 has created a publicly available dataset for future model validation and benchmarking. It attracted participants from 17 institutions across 7 countries and was coordinated with the 35th ISOPE conference, where 10 related papers were presented. The blind test also quantified how well current numerical codes can capture key sloshing responses, including free-surface evolution, hydrodynamic loads and nonlinear flow behaviour.

International engagement and publication impact.
To further strengthen the broader international impact of the activity, we also launched the Special Issue "Sloshing of Liquid Hydrogen Fuel Tanks" in the leading international journal *Ocean Engineering* (https://www.sciencedirect.com/special-issue/10FJLH3815G). At the time of reporting, the Special Issue had closed for submissions, with 18 submissions received and 15 papers still under consideration. This strong response demonstrates sustained international community engagement and shows that the blind test has developed beyond a single conference activity into a longer-term publication and validation exercise.
Broader evidence of community research activity is also reflected in ResearchFish records, with 27 HEC-WSI publications and 24 CCP-WSI publications recorded since the beginning of 2025, alongside the BT5 ISOPE papers and Special Issue activity.

Accelerated computing and industrial relevance.
The accelerated OpenFOAM and multiphysics-coupling outputs further support future industrial workflows by reducing barriers to high-fidelity simulation on modern HPC platforms. This aligns with the UK Industrial Strategy priorities in Clean Energy Industries, Advanced Manufacturing, and Digital and Technologies, particularly through enabling improved digital engineering capability for offshore renewable energy and other engineering sectors.

Digital reach and community engagement.
The wider reach of CCP-WSI activities is also reflected in digital engagement metrics. The CCP-WSI YouTube Channel now has 1,917 views and 50 subscribers, while the CCP-WSI GitHub organisation includes 9 repositories, 114 members, 14 followers and 16 benchmarking test cases.
The combined CCP-WSI, HEC-WSI and SIG-WSI mailing list has 210 members. HEC-WSI currently supports 23 sub-groups, including 8 institutions and 15 projects, with 60 active users from 21 organisations. During this reporting period, the CCP-WSI website received 4,441 page views from 3,162 users over 3,454 sessions, and the WSI Catalogue received 2,086 page views from 927 users over 1,345 sessions.

Wider community activity and future impact pathway.

Future impact will be supported through two upcoming cross-community activities: the 3rd CCP-WSI Hackathon on AI acceleration for WSI simulation codes to be held at the University of Exeter, 13 -15 July 2026., and the Engineering CCP Conference to be held in Oxford, 14-15 September 2026. Together, these events will create opportunities for cross-community exchange on AI/ML methods, accelerated computing, multiphysics coupling, reproducible workflows, benchmark cases and emerging research outputs across engineering-facing CCP and HEC communities. The CCP and HEC-WSI were presented by Deborah Greaves as part of her Inaugural lecture as President of the IMarEST on 28 April 2026 and at the research seminar at the University of Strathclyde on 15 May 2026. Both of these will widen and increase the community engagement.

4. Up to 5 research outputs that create an impact story for your community

The following five outputs together demonstrate the community's progress in advancing reliable, reproducible and scalable computational workflows for wave–structure interaction. They form an impact story linking experimental and numerical benchmark development, community blind-test validation, GPU-enabled CFD acceleration, and emerging AI/UQ methods for WSI applications.

- Wendi Liu, Omar Ahmed Mahfoze, Mayank Kumar, Stephen M. Longshaw, Eduardo Ramos Fernandez and David R. Emerson, Multiscale Universal Interface v2.0: Lowering Barriers to Scalable Multiphysics Coupling, *Computer Physics Communications*.(under review)
- Mayank Kumar et al., Porting OpenFOAM on GPU via modern C++ , ParCFD' 2026 proceedings.
- Scott Andrew Brown et al., A blind comparative study on isothermal sloshing in a circular tank (CCP-WSI Blind Test Series 5), *Ocean Engineering*.(under review)
- L.Zhao, A.G.L.Borthwick and D.M.Greaves, Experimental and Numerical Study of Energy Dissipation of the Phase-Focused Wave Breaking, OMAE 2026-179560, 2026
- T.Y.Zhao, Yeaw Chu Lee and D.M.Greaves, Towards the Uncertainty Quantification of Neural Operators for Wave–Structure Interaction: A Sloshing-Tank Benchmark, OMAE2026-181887, 2026

Together, these outputs show a coherent pathway from experimental and numerical WSI benchmarks to community validation, accelerated CFD software and AI-enabled uncertainty-aware modelling.

5. Workshops and new opportunities*

1) 3rd CCP-WSI Hackathon: AI acceleration for WSI simulation codes
Date: 13–15 July 2026
Location: University of Exeter, Streatham Campus
Status: Registration open / applications in progress; 16 participants have registered so far.

Details: This three-day hackathon will focus on AI-based acceleration of WSI simulation codes, including hands-on training, collaborative code development, and discussions on sustainable, reproducible community workflows.
Cross-community relevance: This event may be of interest to communities working on AI for simulation, accelerated computing, multiphysics coupling, CFD, offshore engineering and scientific software sustainability. It offers opportunities for cross-community exchange on transferable AI/ML methods, code acceleration strategies and reproducible workflows.
Link: https://ccp-wsi.ac.uk/events/hackathons/exeter2026/

2) Engineering CCP Conference
Date: Provisionally 14–15 September 2026
Location: Oxford
Status: In preparation
Details: A cross-CCP engineering-focused conference currently being developed, bringing together communities working on fluid engineering, wave–structure interaction, nuclear thermal hydraulics, turbulence, quantum computing and related computational engineering topics. The event will encourage participation from PhD students and early-career researchers, with opportunities for oral and poster presentations.
Cross-community relevance: This event is specifically intended to support cross-community working between engineering-facing CCPs and related HEC communities. It will provide a forum for sharing methods, software practices, benchmark cases and emerging research outputs across different application areas.

6. Issues and problems*

The PI, Deborah Greaves, PDRA, Tianyang Zhao, Administrator, Lige Zhao, and leadership of the CCP and HEC-WSI moved to the University of Oxford in February 2026. The University of Plymouth remain collaborators with Co-I Yeaw Chu Lee.

CCP Turbulence for the Period 01/10/25 to 31/03/26

Prof. Sylvain Laizet (CCP Turbulence Chair)

1. Background

No change to previous

2. Outputs

Continuous maintenance and support activities: This task is dealing with software sustainability. With a constantly evolving HPC landscape, it is crucial to make sure that the features already available in our flow solvers are optimised, reliable and robust enough to be compatible with the latest versions of libraries and compilers.

Development of a new version of 2DECOMP&FFT in C++ with a multi-backend approach for use on CPUs and GPUs.

On-going work on building a FAIR Data Repository framework for the UK Turbulence Consortium community with InvenioRDM and Ceph.

Release of the version 2.1 of the library 2DECOMP&FFT with new capabilities such as the option to skip directions in the FFT operation allowing for the FFT option to be mixed with finite difference for the resolution of Poisson like problems, possibility to have sine and cosine transforms via a FFTW backends, restore the possibility to have ALL_TO_ALL communication beside the traditional ALL_TO_ALL_V for both CPU and GPUs and several updated on the ADIOS2 backends for the IO.

Adding of a new capability to OPS to handle particle like data structure. This will be the base for the new Lagrangian particle tracking into OPS supported code like SENGA2. The capability is very general and allows also for particle-particle iterations of particle with inertia and it is also used by other CCP communities (i.e. CCC-ParaSolS) for parallelising and porting to GPU Discrete Element Methods solvers.
Development of a visco-elastic solver in Xcompact3d.

3. Research Implications and Impact

The community's flagship Grand Challenge targets the UK's ambition to triple wind energy production in 25 years. As the UK's installed wind capacity grew from 13.6 GW in 2015 to around 30.4 GW in 2024, the UKTC and CCP Turbulence have played a pivotal role in advancing wind engineering research through high-fidelity CFD and AI based methods.

A critical problem they address is inter-farm wake interactions where upstream wind farms reduce wind speed and energy availability for downstream farms by creating large wakes extending up to 100 km, causing economic losses and potential legal disputes between operators.

Their solution involves creating digital twins of real wind farms using high-fidelity simulations at scales from metres to thousands of kilometres, incorporating realistic atmospheric conditions, complex terrain, and resolved turbine geometries.

The intended outcome is a suite of advanced modelling tools essential to the future security of the UK's wind energy production, informing coordinated planning between neighbouring farms, ensuring fair resource sharing, and supporting evidence-based regulatory frameworks. This Grand Challenge maps directly onto at least two of the IS-8 growth sectors. Clean Energy Industries is a priority sector under the UK's Modern Industrial Strategy.

4. Up to 5 research outputs that create an impact story for your community

Report from CCP Turbulence and UK Turbulence Consortium to the CoSeC Community Forum

Outreach video around the use of AI for Turbulence https://www.youtube.com/watch?v=lwedi5eM-14, over 32k views on YouTube.

All the publications from the UK Turbulence Consortium members who used ARCHER2 can be found here: https://www.ukturbulence.co.uk/publications—talks.html.

5. Workshops and new opportunities*

- Final community meeting to be held in London in January 2027.
- CCP Engineering Conference in collaboration with the CCP-WSI community in Fall 2026.
- CECAM Course on HPC and CFD using code_saturne to be held in Barcelona Supercomputing Centre at the beginning of October 2026.
- Contribution to established events like CIUK2026.

6. Issues and problems*

The main problem in the last few months has been the lack of support for OpenSBLI and SENGA+, where little effort has been allocated in terms of CoSeC staff.

Limited options to benchmark our software (at scale) on GPU nodes in the UK.

End of the Tier2 systems in the UK and end of ARCHER2 (Nov 2026), with the new supercomputer planned for early 2028 in the most optimistic scenario.
Lack of clarity about the future of the CoSeC support for CCP projects and lack of clarity about the future of the HEC consortia (after 2026).

CCP-NTH for the Period 01/10/25 to 31/03/26

Prof. Shuisheng He (CCP-NTH Chair), Dr. Wei Wang (CoSeC Project Lead)

1. Background

No major changes to previous submissions.

The Collaborative Computational Project for Nuclear Thermal Hydraulics (CCP-NTH) supports the UK nuclear thermal-hydraulics community through the development, application, and dissemination of advanced computational methods and software. The community brings together researchers from universities, national laboratories, industry, and government organisations to address challenges in reactor thermal hydraulics, turbulence, heat transfer, multiphase flow, and coupled multi-physics simulation.

CCP-NTH activities focus on high-fidelity modelling and simulation, including direct numerical simulation (DNS), robust computational fluid dynamics (CFD), subchannel analysis, and potentially extending to multi-scale/multi-physics coupling approaches. The community also supports the development of benchmarking and validation activities, technical training, and collaboration with international initiatives.

During this reporting period, CCP-NTH further expanded its scope to include fusion thermal hydraulics, recognising the growing importance of thermal-fluid challenges associated with future fusion energy systems. In collaboration with UKAEA, CCP-NTH co-organised the first UK Fusion Thermal Hydraulics Workshop in November 2025, bringing together researchers from fission and fusion communities to identify shared computational and modelling challenges.

2. Outputs

During this reporting period, CCP-NTH delivered significant outputs across high-fidelity simulation, accelerated computing, training, community engagement, and emerging AI-related activities.

High-Fidelity Simulation and Software Development: Development of the community DNS software CHAPSim2 continued, with ongoing improvements targeting nuclear thermal hydraulics and fusion-energy-related applications. Activities included GPU porting and performance optimisation for heterogeneous HPC architectures, development of magnetohydrodynamic (MHD) modelling capability, and extension of immersed boundary functionality for complex geometries and rough-wall heat-transfer studies. These developments support both high-fidelity turbulence research and future fusion blanket thermal-hydraulics applications.
Community-supported research was presented at major international conferences including NURETH-21, UKTC Annual Meeting 2026, and the National Laboratories Research Conference 2025.

Accelerated Computing and Green Computing: A major focus during this reporting period has been the GPU porting and optimisation of the community DNS software CHAPSim2 to support next-generation heterogeneous HPC systems. This work forms part of CCP-NTH's longer-term strategy to enable high-fidelity turbulence and heat-transfer simulations at scales relevant to advanced nuclear systems and future fusion-energy applications. The GPU acceleration strategy is based on OpenACC and targets efficient vectorisation of the large computational kernels within CHAPSim2. Significant progress has been achieved during this reporting period, including successful GPU porting of key numerical operations such as interpolation, derivative evaluation, and divergence computation. Performance benchmarking indicates that a single NVIDIA H100 GPU node can provide computational performance equivalent to approximately 32 ARCHER2 CPU nodes for CHAPSim2, highlighting the significant potential of heterogeneous GPU-accelerated HPC for high-fidelity turbulence simulations. These activities directly support the UK's broader accelerated-computing and digital research infrastructure priorities while also contributing to greener computational workflows through improved hardware efficiency, reduced simulation turnaround times, and lower energy consumption per simulation campaign.

AI and Data-Centric Activities: CCP-NTH continued exploratory activities related to AI and machine learning applications in nuclear engineering and thermal hydraulics. This included ongoing review and assessment of AI/ML methodologies relevant to turbulence modelling, surrogate modelling, reduced-order modelling, and uncertainty quantification. The community also strengthened its focus on FAIR data principles through benchmarking activities and preparation of high-fidelity datasets for open dissemination and future AI/ML applications.

Community Engagement and Training: CCP-NTH delivered a wide range of community activities during this reporting period, including: 1) CHAPsim2 weekly developer update meetings, 2) two research days, 3) webinars, 4) software training activities, 5) workshops. All these have been reported in the CoSeC Matrix report.

The first CCP-NTH Fusion Thermal Hydraulics Challenge Day, co-organised with UKAEA, attracted over 50 participants and established a new cross-community activity bridging fusion and fission thermal-fluid research. Additional activities included Code_Saturne training,

support for NURETH-21 participation, and international HPC-related turbulence-modelling training delivered in collaboration with the Barcelona Supercomputing Centre.

3. Research Implications and Impact

The outputs from CCP-NTH during this reporting period contribute directly to strengthening UK capability in advanced nuclear-energy modelling and simulation.

Development of high-fidelity simulation capability through CHAPSim2 supports national priorities in advanced reactor development, reactor safety, and future fusion-energy systems. The extension of DNS and MHD capabilities provides important benchmark-quality data for turbulence, heat transfer, and coupled multi-physics phenomena under conditions relevant to advanced reactors and fusion blanket technologies.

GPU porting activities contribute to the UK's broader strategy in accelerated computing and digital research infrastructure by enabling next-generation scientific applications on emerging heterogeneous HPC platforms.

The expansion into fusion thermal hydraulics creates new opportunities for collaboration between fission, fusion, HPC, and AI communities. This aligns with current UK priorities in clean energy, sovereign computational capability, and advanced engineering for net-zero technologies.

CCP-NTH training, workshops, and open community activities continue to support skills development, knowledge exchange, and workforce capability across academia, national laboratories, and industry. These activities contribute to maintaining and growing UK expertise in computational engineering, nuclear thermal hydraulics, and scientific computing.

4. Up to 5 research outputs that create an impact story for your community

(1) GPU Porting and HPC Performance Development of CHAPSim2: CCP-NTH continued development of GPU-enabled DNS capability through porting and optimisation of CHAPSim2 for heterogeneous HPC systems. This work supports future large-scale turbulence and heat-transfer simulations while improving computational efficiency and reducing energy consumption.

(2) Expansion into Fusion Thermal Hydraulics: CCP-NTH and UKAEA co-organised the first UK Fusion Thermal Hydraulics Challenge Workshop in November 2025, establishing a new interdisciplinary activity focused on computational challenges for future fusion-energy systems. This expanded CCP-NTH's scope beyond traditional fission applications and initiated new collaboration opportunities between thermal-fluid, HPC, and fusion communities.

(3) Reactor Vessel Auxiliary Cooling System (RVACS) Benchmarking: Community members completed benchmarking studies of RVACS natural convection flows using DNS and RANS methodologies. Associated datasets are being prepared for open dissemination, supporting FAIR data principles and future validation activities for thermal-hydraulics codes.

(4) International Visibility through NURETH-21 and UKTC: CCP-NTH-supported researchers presented multiple contributions at NURETH-21 and the UK Turbulence Consortium Annual

Meeting, covering DNS, MHD, cost-effective modelling, and advanced reactor simulation. These activities strengthened the international visibility of UK computational thermal-hydraulics research and reinforced collaborations with academic and industrial partners.

5. Workshops and new opportunities*

Planned Activities (Next 12 Months)

- CCP-NTH and UKFN SIG-NTH Annual Technical Meeting – June 2026, Manchester
- AI for Nuclear Thermal Hydraulics (AI4NTH) Summer School – July 2026, Daresbury Laboratory
- CCP-NTH Research Days – regular community research and developer meetings
- CHAPSim2 Developer Update Meetings – weekly
- Potential follow-on Fusion Thermal Hydraulics Workshop in collaboration with UKAEA – Nov 2026

New Opportunities:

- Potential participant in Computational Centre of Excellence (CCE)
- Potential participant in National Supercomputing Service (NNSS)

6. Issues and problems*

Access to Modern GPU Development Infrastructure: While national HPC systems provide substantial production-scale computing capability, there remains limited immediate access to modern GPU hardware for interactive software development, debugging, profiling, and rapid testing workflows. Efficient GPU porting and optimisation activities often require responsive access to advanced accelerator systems outside of traditional batch-production environments. The lack of readily accessible next-generation GPU development platforms can significantly slow software development cycles, performance tuning, and portability testing for community codes.

Long-Term Sustainability and Strategic Continuity of CCP Activities: The current uncertainty surrounding the long-term structure and continuation of CCP funding and support beyond March 2027 presents challenges for strategic planning, community development, and long-horizon software sustainability activities. Many CCP-supported activities, including community software development, benchmarking programmes, training pipelines, and cross-institution collaborations, inherently require multi-year continuity. Greater clarity regarding future support models would significantly assist long-term capability planning and retention of community expertise.

Alignment Between AI Initiatives and Domain-Specific Scientific Support: CoSeC and wider UKRI activities increasingly promote AI adoption within scientific computing and engineering research. However, there remains a gap between high-level AI strategy and the availability of sustained, domain-specific technical support for communities such as CCP-NTH. In particular, effective application of AI/ML methods to computational thermal hydraulics requires close integration between AI expertise, HPC workflows, numerical methods, turbulence modelling, and domain-specific validation practices. Stronger alignment between AI-focused initiatives and established scientific-computing communities would help accelerate meaningful and scientifically robust adoption of AI methodologies.

Increasing Software Maintenance and Community Support Demands: As CCP-NTH activities expand into areas such as fusion thermal hydraulics, GPU-enabled HPC, and AI-enhanced simulation workflows, the demands associated with software maintenance, user support, training delivery, and benchmarking activities continue to increase. Sustained support for research software engineering and community coordination remains essential to maintain long-term impact and software sustainability.

Tomographic Imaging

CCPi for the Period 01/10/25 to 31/03/26

Prof Philip Withers (CCPi Chair), Prof William Lionheart (CCPi Co-Director), Dr Jakob Jorgensen (International), Dr Edoardo Pasca (SC/STFC) and Dr Martin Turner (CCPi Secretariat)
1 May 2026

1. Background

The computational collaborative project in tomographic imaging (CCPi) was initiated in 2012 to support the UK nonclinical computed tomography (CT) community with the aim of: 'Developing software and the necessary training to increase the quality and level of information that could be gleaned from X-ray projection data.' Specifically, three suites of open-source software tools have been developed by CCPi in response:

1. simulation software for calibration, training, experiment planning, generation of data for development of methods and AI tools; and
2. software for pre-processing of raw CT data and reconstruction able to reconstruct a 3D/4D volume images from both standard and 'sub-optimal' datasets; and
3. quantification techniques to extract relevant quantities from 3D/4D data, such as Digital Volume Correlation.

This extensive python ecosystem supports CT users across a wide range of imaging devices including lab X-ray, national mid-scale research facilities and synchrotron X-ray and neutron CT. Our CoSeC support enables us to develop, maintain, and promote this CCPi Core Imaging Library (CIL) (last main release CIL v 25) as well as a range of other related software; notably interactive visualisation and the iDVC (Digital Volume Correlation) code initiated as a result of CCPi funded international visits.

2. Highlights for the current reporting period

We report here on several community engagement events, over the reporting period, spanning the multiple CCPi supported codebases, all increasing the user and developer base. This participation exceeds the original CoSeC grant targets and those outlined in the 2018 EPSRC X-Ray CT roadmap.

In the past period we *sponsored, assisted in running and supported the following events*:

- IBSim-4i, **20-23 October 2025**, held at the IoP London

• CT Public Engagement @ Daresbury Laboratory Public Access Day **October 28, 2025** Part of the major Public Access Day
• Mantid User Workshop, **6-7 November 2025** CIL code integration
• Workshop on CT and DVC – with France, Bordeaux on **12 November 2025**
• Autumn CIL Hackathon; **18-21 November 2025** ("CIL CT Data Reader Hackathon")
• CoSeC Conference **3 December 2025** with CIL presentations and posters
• CIL User Meeting, **27-30 January 2026**, Rutherford Appleton Laboratory
• CIL training at the AI hackathon for women in mathematical sciences **February 18, 2026**
• Future AI Conference, 2026, a joint event between NVIDIA and the School of Computer Science & Engineering **4 – 5 March 2026** Bangor University
• Symposium on AI and Reconstruction for Biomedical Imaging, **9-10 March 2026** CCPi supporting CCP SyneRBI; followed by hackathon on ML **11-12 March 2026**
Future AI Conference **4-5 March 2026** at Bangor with invited CCPi talk with student-facing hackathon **6-7 March 2026**
• Attendance at Creating a New Reality: A Sustainable Digital Transformation **22 – 23 April 2026** Department of Physics, University of Oxford, OX1 3PU

During this reporting period we also integrated into codebase and publicised outputs from the *CCP Bridging Funding FY24-25 Additional Components* (**March-May 2025**): Update of datasets are now within the Zenodo archive and being used; also, bespoke training and presentations on this codebase along with the rest of the CCPi (Core Imaging Library www.ccpi.ac.uk/CIL) portfolio.

Outreach: continual collaboration with the Mantid Imaging team (ISIS), the CIL team continue to exploit Tomography public engagement activities, which includes at various conference stands and at the DL open day in **November 2025.**

-A fortnightly CCPi Show-and-Tell online meeting is organised to strengthen the community bonds and foster exchange of ideas and information (in the period 9 short talks were given by users and developers; as well as 2 multi presentation sessions from the main Hackathon outcomes).

-A new IoP sponsored series of talks has commenced: Webinar series in IBSim: "X-ray CT in academia, government, and industry: Current and future systems and applications" **January 20, 2026** and **15 April 2026**

- *Strengthened links with our USA associated network NoCTURN,* online presentations **19-20 November 2025** workshop and face-to-face meeting **12-14 May 2026**

Standards and support for Dimensional-XCT: Attended and voted on BSI / ISO standardisation WG10 meetings. **2-4 March 2026** in Berlin

Training: The network carries out its own training courses on the main developed software; but also collates and advertises community training; notably linked through the NXCT.ac.uk, and the

University of Manchester at Harwell; as recommended from the 2018 EPSRC X-Ray CT roadmap report.

CIL Software: In the reporting period CIL has the annual 1 stable release.
iDVC software: Version 26.0.0 of the iDVC digital volume correlation software has been released.

3. Overview of work relating to accelerated computing

We have four outcomes on the current proposal that are all progressing, with specific software development coding outputs. Three are focussing on acceleration and optimisation:

1. Utilise heterogeneous computing including new GPU architectures for increased software efficiency;
2. Incorporate fundamental algorithmic design including new optimisation methods;
3. Enable code optimisation for environmentally sustainable computational resources;

A further outcome actively has been successfully utilising the STFC Cloud environment.
4. Develop training platforms and learning tools based on cloud resources;

4. Current plans, developments, or specific applications of AI

Code and work from a workshop and hackathon on Efficient Integration of SIRF/STIR/CIL with Pytorch, to enable the better and more informed use of AI libraries within the CIL pipeline. The main outcomes:

1.Enable the integration of AI/ML tools across the full XCT pipeline process via agnostic data containers, see GitHub site
2.Strengthen integration with gVXR for the generation of labelled training data for AI methods training.
3.Plug and play methods, such denoisers, already publicly available, such as on DeepInv.

A series of AI events have supported this including a follow-on Symposium on AI and Reconstruction for Biomedical Imaging with hackathon, **9-10 March 2026** (CCPi supporting CCP SyneRBI)

An NPRAISE grant was awarded to deal with AI for specific CCPi issues – funding to support RTP development in AI and ML through our project "AI Integrated High-Speed Imaging for Manufacturing"; welcoming Evelien Zwanenburg (Warwick) formally to the team **1 September 2026 - 31 August 2027**

5. Up to 5 research outputs that create an impact story for your community from the reporting period

Built upon the simulation software awards and publication list; with a full list of 13 papers in the last 12 months: full report at end of year.

Two related new grants have been awarded that connect the reconstruction with added Intelligence modes:

- UKRI grant "AC/DC – Accessible CT Data Compression", joint with UoCambridge and UoPortsmouth
- NPRAISE grant "AI Integrated High-Speed Imaging for Manufacturing"

6. Workshops and new opportunities

A list of future workshop and conferences with a participation of CoSeC or CCPi:
• SC4RC 2026, **4-8 May 2026**
• CGVC (Computer Graphics and Visual Computing – UK) co-located with EuroVis at Nottingham **8-12 June 2026**
• Dimensional-XCT Conference – metrology focussed project in liaison with NPL: **16-17 June 2026** including training on CCPi gVirtualXray system
• UoM at Harwell hosting the 9th Advanced in X-Ray Imaging Workshop, at RAL **23 June 2026**
• Open Day PE activities "Family Day" for CCPi code, **29 June 2026**
• ICTMS at Manchester, 6-10 July 2026; with CCPi special session on **7 June 2026** and training on Friday **3 July 2026**
• **1-4 September 2026** NanoTec26 Conference in Manchester
• ToScA International Europe, in Greece; **2-4 September 2026**
• IMA 5th Inverse Problems Conference **8-10 September 2026**
• RSE Conference **9-11 September 2026**
• 27th IUCR Congress **11-18 September 2026** in Calgary, with the microsymposium on X-ray ptychography from 2:30 to 5:00pm **16 September 2026**
• NOBUGS'26 **21-25 September 2026**

A new XCT Roadmap is planned with activities and milestone set **March 2027**. Previous roadmap was available, on the EPSRC website (2018 EPSRC X-Ray CT roadmap) and has informed projects over the last 8 years. Activities planned:
• Two Online Surveys for Future XCT uses and needs; one for the community and the other for the industrial contacts
• One-to-One interviews regarding specific contacts from survey responses.
• Three Town Hall meetings; one virtual; and the other two based in London and in Manchester.
• Report to be edited and published on a UKRI website dictating future vision including grand challenges.

7. Issues and problems*

Funding is uncertain, although there has been some external grant success – see above. We continual to search for other sources of income including from SSI funds to support software development and more importantly maintenance.

Work has been ongoing for the transfer of the Website to a new server and updated style-file which is now stable and we hope to build with possibly cross-link to other CCPs.

STFC Cloud Infrastructure, which has been in the past very useful for user training, hackathons as well as testbed setups; has stabilised and will be continuing to apply for time.

A No-cost Extension for the CCPi Network; was approved until the end March 2027 is useful for continuity but not for support. We find specific admin and network budget finance support incredibly useful.

CCP-SyneRBI for the Period 01/10/25 to 31/03/26

Prof Kris Thielemens (CCP-SyneRBI Chair), Evgueni Ovtchinnikov (CoSeC Project Lead)

1. Background

No changes to previous.

2. Outputs

2.1 Online training for SIRF

An online-only training day for starters with the SyneRBI main software package SIRF had ~40 attendees ranging from MSc students to ECRs.

2.2 PET Rapid Image Reconstruction Challenge 2 (PETRIC2)

We organised PETRIC2, a sequel to the previous PET Rapid Image reconstruction Challenge (PETRIC, ran in 2024-2025). As with PETRIC, our primary aim was to stimulate research into the development of fast PET image reconstruction algorithms applicable to real world data, and we focused on reconstruction in a Maximum A Posteriori setting. The main difference compared to PETRIC was that the data was much noisier, and the software was updated for faster performance.

The task was to reach a solution which would be close to the converged target image (in terms of standard clinical measures) as quickly as possible (as measured in terms of wall clock time). This task therefore required a balance between algorithm design and implementation optimisation. Participants had access to phantom data acquired on a range of clinical scanners for testing their algorithms.

We had 5 teams submitting, with 14 different algorithms, although more teams registered for the challenge. All data, evaluations and submissions are available from github.com/SyneRBI/PETRIC2/wiki/Awards-and-results.

2.3 Domain-adaptation of image reconstruction algorithms

We continue, in collaboration with CCPi, to develop, adapt and test the application of various optimisation algorithms to the image reconstruction problem. These are now implemented in the Core Imaging Library (CIL) and maintained by CoSeC.

2.4 Integration of PET and MR Raw data into an open database and management platform

Medical image data is commonly saved in widely accessible DICOM or NIFTI format. Raw data handling is much more challenging as there is little support apart from vendor-specific proprietary software tools. Together with a team from the Advanced Research Computing (ARC)

centre at UCL and the German metrology institute PTB, we developed open-source plugins for XNAT, an open-source imaging informatics software platform, see github.com/SyneRBI/xnat-mrd and github.com/SyneRBI/xnat-interfile.

2.5 Progress on a standard for PET Raw data

SyneRBI continues to contribute towards the development of a standard for PET raw data called PETSIRD, an effort coordinated by the Emission Tomography Standardization Initiative (ETSI), see etsinitiative.org/. The 4th ETSI hackathon was held in Japan with about 40 attendees in-person. We are working towards establishing a test protocol and data-set, converters from existing vendor formats, and release of the standard end 2026.

2.6 Symposium on AI and Reconstruction for Biomedical Imaging

This two-day symposium held on 9-10 March 2026, featuring invited internationally leading researchers covering recent advances in AI and image reconstruction for biomedical imaging, was intended to enhance UK and international networking, research progress and education in this important area. We had 139 in-person and 31 online attendees. The symposium included a dedicated session with presentations of the winning teams of the PETRIC2, see above.

2.7 Hackathon on advancing STIR (Software for Tomographic Image Reconstruction)

This 2-day hackathon brought together 30 researchers and industrial representatives using the open-source STIR software for PET and SPECT image reconstruction, covering several aspects, including:

- Improving GPU performance
- Reconstructing measured PET data
- Using PET Monte Carlo software (SimSET) with STIR

The hackathon led to our first reconstructions of SimSET simulated data for recent Long Axial Field of View (LAFOV) PET scanners, data from the Siemens Vision 600 PET/CT scanner, as well as a skeleton for GPU-enabled acquisition modelling for SPECT.

2.8 Hackathon on Software for Machine Learning Approaches for Reconstruction in Biomedical Imaging

Associated to the AI-RBI symposium, there was a 2-day hackathon on software for machine learning (ML) approaches in biomedical imaging with specific emphasis on the SyneRBI package SIRF and the DeepInverse open-source software, building on our previous work on integration SIRF with PyTorch. The participants worked on:

- Optimisation of GPU computation and data copies in STIR and SIRF.
- Adapt the open-source CASToR image reconstruction software to call PyTorch regularisers.
- Implementation of “plug-and-play” methods: using learned regularisers from DeepInverse into CIL algorithms using SIRF acquisition models.
- Implementation of ML-based optimisation algorithms from DeepInverse to use the SIRF acquisition models directly.
- AI-tools allow commercial MRI scanners to acquire only 25-30% of a full dataset, resulting in shorter patient acquisition time and more efficient hospital workflows. However, the AI-tool and the risk of hallucinations is not fully understood. We worked

with NHS St George's hospital to create an alternative reconstruction algorithm for the reduced dataset for QC.

The hackathon (45 in-person and 5 online attendees) resulted in multiple Pull Requests to 5 different open-source packages. Progress can be tracked at github.com/orgs/SyneRBI/projects/13/.

3. Research Implications and Impact

Our main impact in this reporting period was related to PETRIC2. Aside from making SyneRBI and our software output known to a wide international audience, the main impact relates to the demonstration of feasibility of using advanced reconstruction methods for challenging data within clinically acceptable processing times. Winning submissions were able to reconstruct within the clinically motivated required limits set by the challenge within 1-4 minutes, with further optimisation of the software in progress. This reduces computational load dramatically compared to current "reference" algorithms.

In addition, we continue to make progress towards enabling FAIR data access via open standards and software. For instance, our work is currently under consideration for a proposed Data Platform for the National PET Imaging Platform (NPIP).

One of the outcomes of the AI-RBI hackathon is a study with St George's NHS trust and PTB to study time-reduced acquisition MRI protocols and compare vendor AI-assisted reconstruction with variational approaches to prevent patient recalls is under way.

4. Up to 5 research outputs that create an impact story for your community

The aims, set-up and results of our previous reconstruction challenge PETRIC were published in

Casper da Costa-Luis, Matthias J. Ehrhardt, Christoph Kolbitsch, et al. 'PET Rapid Image Reconstruction Challenge (PETRIC)'. *Frontiers in Nuclear Medicine*. https://doi.org/10.3389/fnume.2026.1770002.

As far as we are aware, PETRIC was the first open challenge on image reconstruction in nuclear medicine. Its output includes phantom datasets, reconstruction software, independent evaluation of algorithms of different research groups, but also an open-source framework for future challenges.

PETRIC2 provides a snapshot of current state-of-the-art image reconstruction algorithms, with several different approaches submitted by participants and their evaluations are available from github.com/SyneRBI/PETRIC2/wiki/Awards-and-results. Importantly, all submitted algorithms were made open-source by the participants and can be therefore be used (or further developed) by other researchers. We are aware of several avenues of further research that will be pursued by some of the participants.

The PETSIRD proposed standard continues to create excitement and considerable community engagement. It is still in progress but was presented at one of the major international conferences.

> Thielemans, K., Asma, E., Cook, M., et al.., 2025. Final Draft of PETSIRD v1.0: A Proposed Standard for PET Raw Data, in*: 2025 IEEE Nuclear Science Symposium, Medical Imaging Conference and Room Temperature Semiconductor Detector Conference*. https://doi.org/10.1109/NSS/MIC/RTSD57106.2025.11287540

The XNAT plugins see github.com/SyneRBI/xnat-mrd and github.com/SyneRBI/xnat-interfile will allow XNAT users to store MR and PET raw data, where meta-data is extracted and made visible to the user. This is an important step to be able to apply advanced image reconstruction techniques to clinical data in a transparent and easy-to-use environment.

5. Workshops and new opportunities*

- EFOMP workshop at ECMP 2025: Image Reconstruction for Quantitative Molecular Diagnostics and Radionuclide Therapy, Valencia, Spain, 23 September.
- Workshop on Sustainability in Medical Imaging and associated hackathon, Edinburgh, 5-6 October
- STIR User's group at IEEE MIC, Granada, Spain, 12 November
- ETSI hackathon at IEEE MIC, Granada, Spain, TBC

6. Issues and problems*

The main stumbling block affecting our software development remains the installation of SIRF and its pre-requisites under various Operating Systems. While we provide a Virtual Machine and docker containers, this is still a hurdle for many users. We also face issues with some of our dependencies have lacking active maintenance. A particular example is Gadgetron which we use for some of the MRI processing. In the long term, we will have to replace Gadgetron.

Quantum Computing

CCP-QC for the Period 01/10/25 to 31/03/26

Prof. Viv Kendon (CCP-QC Chair)

1. Background

“No changes to previous”

CCP-QC was started in 2019 with a remit to bring about close co-operation between other CCPs and the quantum computing community, rather than build a separate computational community for quantum computing. CCP-QC aims to:

- Build an active research community encompassing CCP members interested in enhancing their simulations by adding quantum computing capability to their code, and quantum technology researchers working on applications of quantum computing to simulations;
- Generate small projects supported by CoSeC staff time to develop methods appropriate to specific applications, leading to proof-of-concept demonstrations on early quantum hardware. This will also develop capacity in CoSeC for quantum computing;
- Collaborate with the National Quantum Computing Centre (NQCC) and the Quantum Computing (QCi3) Hub in developing early applications of quantum computing;
- Provide training in quantum computing for researchers who are expert in computational science but lack quantum computing knowledge;
- Support career development of early career researchers through subsidised meetings, annual awards for best presentation, and a pairing scheme to link those working in computational science with those working in quantum computing and quantum algorithms;
- Promote cross-CCP networking to share knowledge on early applications of quantum computing, enabling the widest possible early adoption of quantum enhanced computational science;
- Provide information on early quantum computing applications in academic research to the wider community through their website maintained for the life of the CCP. The website will advertise contact details and opportunities to join the community through meetings, training days, and signposts for collaboration.

CCP-QC does not aim to develop or curate its own body of code, rather, any code developed will belong to the CCP community for that application. Pointers to those applications, and information about what works and why will be available on the website, to guide those developing further applications.

2. Outputs

Supported by CCP bridge project funding, the following work packages have continued to run in parallel:

1. Lattice Boltzmann in the Computational Engineering Theme - CoSeC staff member Zhengliang Liu has run simulations of a quantum lattice Boltzmann algorithm and published the results in a journal article in Frontiers in Mech Eng Jan 2026. This work package has now ended, but workshops on quantum algorithms for fluid simulation continue (see upcoming events section).

2. Green's functions formalism for electronic structure within the Computational Materials and Molecular Science Theme – the journal club continued until the end of the period, and there are plans to transfer the online meetings to the QCi3 Hub, which has a task on quantum algorithms in chemistry and many body dynamics. Useful discussions were held with experimentalists at Strathclyde who run Fermi gas microscopes, and this will feed into the CECAM workshop later this year (see upcoming events section). Work continued in collaboration with CCP9 (Phil Hasnip) on CASTEP matrix preconditioning using quantum annealing, with simulations of a proof-of-concept implementation that may lead to a publication. This work package has now ended, and both RSEs have left for other jobs (one to NPL data science and the other to industry).

3. State preparation and benchmarking within the Computational Mathematics Theme – PDRA Steph Foulds (Strathclyde) has visited RAL/Kathryn Lund (Comp Maths), this work package continues, as Steph is funded from other grants, and the start was delayed by maternity leave.

4. Resource cataloguing for quantum applications – this has also been delayed by maternity leave and we are only at the initial contact stage.

Other activities in this time period include participation in CIUK 2025 and continuing to compile the special issue from the talks given at the Royal Society Discussion Meeting in October 2025. We also ran a round of travel and workshop funding (see upcoming events).

3. Research Implications and Impact

The work on Green's functions and quantum simulation methods for materials chemistry aligns with the first milestone in the UK Government Quantum Technology Mission One (quantum computing) roadmap and is specifically identified in the CCP-QC grand challenges as relevant for all of the CCP communities with simulations involving DFT or related calculations. Beyond this, matrix preconditioning comes up in multiple domains, including high energy physics and radio astronomy – results here potentially have wider impact for these and other domains. Fluid simulation is another important area where any advantage gained from quantum algorithms can have a big impact across many areas of engineering, from aerospace to weather forecasting. The impact is a little further in the future than for materials chemistry but will require more work to overcome the challenges of solving nonlinear PDEs in a quantum setting.

4. Up to 5 research outputs that create an impact story for your community

Fluid simulations:

Quantum Lattice Boltzmann Method based on linear equilibrium distribution functions Zhengliang Liu, John Benzi, and David R. Emerson, Frontiers in Mech Eng 11:1717775 2026 DOI:10.3389/fmech.2025.1717775

Continuum limits of Lazy quantum walks, Lara Janiurek and Viv Kendon, J Phys A Math Theor, DOI:10.1088/1751-8121/ae6d52 https://arxiv.org/abs/2512.17755

Lazy Quantum Walks with Native Multiqubit Gates, Steph Foulds and Viv Kendon, https://arxiv.org/abs/2511.21608

Condensed Matter:

Topical Review on quantum annealing and condensed matter physics, Viv Kendon and Nicholas Chancellor J Phys CM, 38, 143005, 2026 https://arxiv.org/abs/2602.09149

5. Workshops and new opportunities*

QCFD workshop Manchester, 31st April - 1st May. 20 attendees, including new early career researchers who have not been to previous events. Interesting talks on new research directions. Planning two more workshops by end of CCP-QC funding (Mar 2027) and one more under QCi3 Hub funding after this: please get in touch to be added to the contact list for these.

Supporting **Summer School in the Isle of Skye** on quantum computing 25-29 May 2026 to provide early career training in quantum computing and algorithms.

Quantum Algorithms meeting Warwick 5th June after the CoSeC Community Forum, to provide cross-application survey of development and generate collaboration opportunities for common algorithms across application areas. https://ccp-qc.ac.uk/qalg/

CECAM workshop on "Tackling the Many-Body Problem in Condensed Matter with Quantum Computing" Glasgow 1-3 July, co-sponsored with CCP9, PsiK, and CoSeC. https://ccp-qc.ac.uk/ws_mb/

Co-sponsoring with QCi3 Hub on Materials and Chemistry – working group meeting planning underway for later this year. Please get in touch to be added to the contact list for this.

Workshop funding supporting events co-sponsored by CCP-QC run by others:

- Northern Quantum meetings, April (Leeds) + September (Liverpool);
- 7th MACSMIN (Mathematics and Computer Science for Materials Innovation) in Liverpool (April);
- Newcastle Newton-Q workshop (September).

QRALly Computational Maths workshop Cosenor House 23+24 September, co-sponsored with CoSeC and the NQCC.

Co-sponsoring **CCP-WSI Fluid simulation workshop** (Autumn, tbd).

6. Issues and problems*

Delayed scheduling of the Quantum Algorithms meeting (5th June) due to crowded events diary. This now falls just past the end of the original CCP-QC grant no-cost extension, causing some cash flow issues, hopefully now resolved.

Scarcity of current funding and uncertainties over future funding are affecting CCP-QC along with all CCPs, making planning difficult at a time when quantum computing is advancing rapidly. This includes the pressures on STFC funding affecting current and future CoSeC provision of support. Cross-cutting efforts to develop quantum algorithms that can be integrated into future HPC are being delayed, damaging UK competitiveness in this area.

NEW COMMUNITIES' REPORT

CCP-volumeEM for the Period 01/10/25 to 31/03/26

The Collaborative Computational Project for Volume Electron Microscopy

Dr. Martin Jones (CCP-volumeEM Chair)

1. Background

No changes to text previously submitted

2. Outputs

In **WP1**, our inaugural community meeting was held at the Francis Crick Institute in November 2025, with a total attendance of around 80 (40 in person, 40 online). There were a range of talks from vEM practitioners, software developers, and talks from CCP-EM, CCP4 and CCP-NC, covering the full range of stakeholders in CCP-volumeEM activities. The results from our community survey were presented, alongside an overview of our draft roadmap and breakout sessions to discuss various topics relevant to the community. The full report from the event is available at https://www.ccp-volumeem.ac.uk/annual-ccpvolume-em-community-meeting. The community's visibility has been enhanced with a website (https://www.ccp-volumeem.ac.uk/), as well as increasing activity on our LinkedIn and BlueSky channels. A "show-and-tell" series was started in February 2026 (https://www.ccp-volumeem.ac.uk/showandtell) where speakers present webinars on topics of interest to the bioimage analysis community. Recordings of these webinars, along with recordings of talks at the November community meeting, are made publicly available on our YouTube channel (https://www.youtube.com/@CCP-volumeEM), and, where relevant, materials are added to Zenodo (https://zenodo.org/communities/ccp-volume-em). Efforts have been made to further integrate with the CCP-EM community, since the frontiers of the two communities are beginning to overlap in areas such as in-situ imaging, cryo electron tomography and correlative light and electron microscopy. CCP-volumeEM was presented as an invited talk at the CCP-EM Spring Symposium, and we continue to work closely with the volume EM community initiative, ensuring continuing close collaboration with the broader community of microscopists and end-users.

In **WP2**, development work has focused on three main areas. An exemplar workflow to incorporate Next Generation File Formats (NGFF) into stitching and registration workflows has been ongoing (https://github.com/ccp-volume-em/muvis-align) with deployments via Jupyter notebooks and a napari plugin. Developers on this project have been heavily involved in the NGFF community, contributing to broader discussions and standardisation efforts that will benefit the whole bioimaging field. Efforts to improve the accessibility of complex software ecosystems via containerisation are ongoing, with a range of common tools available at https://quay.io/organization/rosalindfranklininstitute. Contributions have also been made to the best-in-class generalised vEM AI segmentation platform (https://github.com/volume-em/empanada-napari), updating the system to current versions of key packages and adding

NGFF compatibility. In parallel to these main development strands, best practice guidance has been shared (https://ccp-volume-em.github.io/guide/) to help the community adopt cutting-edge technologies more easily.

In **WP3**, a hackathon was held at EMBL-EBI, focusing on NGFF in vEM workflows. The participants came from a wide range of backgrounds, from non-developer vEM practitioners, through bioimage analysts, NGFF specialists, CCP-EM members and industry representatives. The outcomes included steps towards providing more straightforward integration of NGFF tooling into the napari platform, integration of NGFF into existing plugins, cross-CCP coordination of best practice, and end-user requirement specification via a submitted user-story (https://github.com/ome/ngff/pull/343#issuecomment-4054132101).
An in-person 5-day training course for CLEM image analysis has been planned for Nov/Dec 2026 (https://www.crick.ac.uk/whats-on/image-analysis-for-correlative-light-and-electron-microscopy-clem) and two online training courses (using STFC's ada VM system) are planned for summer/autumn 2026, one for the napari platform, and one for the empanada AI segmentation plugin.

3. Research Implications and Impact

Support by CCP-volumeEM in modernising the empanada napari plugin has been crucial in keeping the software compatible with evolving requirements, at a time when primary developer effort has been unfortunately limited due to personnel turnover at the principal development lab. The strategies learned in doing this have added to a growing knowledgebase that will be a valuable resource for future development of a range of other plugins. Ongoing involvement with the broader NGFF community ensures vEM-specific requirements are visible and integrated into the rapidly progressing development of data and metadata standards. Creating stronger links between the various stakeholders in the vEM community has enabled much more efficient transfer of information regarding end-user requirements, developer best-practice and community awareness of cutting-edge tools.

The adoption of cloud-native next generation file-formats, containerised workflows and AI methods allows us to prepare the volume EM community for the diversification of scientific computing infrastructure used in bioimaging, providing a natural route into the use of cloud computing and national computational facilities, which will play a crucial part in the future of bioimage analysis, both in terms of the absolute scale of available compute, and also in the democratisation of access to scientific insights from rich vEM datasets beyond the well-funded data generating institutes themselves.

4. Up to 5 research outputs that create an impact story for your community

Our efforts have focused largely on engaging with the community and provided curated and persistent materials to support end-users and developers. Some of these outputs include:

- CCP-volumeEM event report https://www.ccp-volumeem.ac.uk/s/3rd-November-Meeting-Summarydocx-Google-Docs.pdf

- CCP-volumeEM GitHub organisation: https://github.com/orgs/ccp-volume-em/repositories
    - Including muvis-align NGFF-capable stitching and registration toolkit
    - Community good practice guide
- Show and Tell webinar series https://www.ccp-volumeem.ac.uk/showandtell)
- Contributions to the modernisation and maintenance of the napari empanada plugin (primary developers: Narayan lab, NIH, USA) https://github.com/volume-em/empanada-napari
- Development and testing of common software ecosystems as Docker containers https://quay.io/organization/rosalindfranklininstitute

5. Workshops and new opportunities*

- (TBC) Hackathon (ontologies), Bristol, Autumn 2026
- (TBC) CCP-volumeEM community meeting, Nov 18th, York Railway Museum
- Image Analysis for Correlative Light and Electron Microscopy (CLEM), Francis Crick Institute, London, 30th Nov – 4th Dec

6. Issues and problems*

- Uncertainties over the future of CoSeC/CCP activities has caused a bit of concern – we're actively looking at various funding possibilities (and were planning to anyway, of course), but more clarity over the future of CoSeC would be appreciated when possible.
- Future funding of staff time for community management is likely to be crucial since this will be much harder to acquire further funding for than individual events etc.

CCC-ParaSolS for the Period 01/10/25 to 31/03/26

Collaborative Computational Community in Particulate Solids Simulations

Dr. Kevin Hanley (CCC-ParaSolS Chair)

1. Background

No changes to previous.

2. Outputs

Technical training has been a major focus during this six-month period. This has been delivered at three hybrid Network Events, building on the training delivered at the first Network Event in May 2025 on running three open-source discrete element method (DEM) codes:

—— *Network Event 2 (Abingdon: October 2025)* ——
The second three-day Network Event took place in Oxfordshire. This event included two days of training delivered by experts from EPCC on the use of HPC with ARCHER2 as an exemplar and running a DEM simulation on ARCHER2 with LAMMPS (& the Granular package). This Network

Event was very successful, attracting ~25 in-person attendees and 5–10 online attendees each day.

—— *Network Event 3 (Manchester: January 2026)* ——
This two-day event, hosted by the University of Manchester, focused on the use of AI in the simulation of particulate solids. Four invited speakers presented the state of the art in this area, the recordings of which are accessible through the event webpage. The second day contained workshop/tutorial sessions on automated simulation calibration and deep learning. More than 30 people attended in person with several more online.

—— *Network Event 4 (Belfast: March 2026)* ——
This most recent three-day event was organised jointly with the ON-DEM COST Action at Queen's University Belfast. 30–40 in-person attendees each day contributed to discussions on developing a common open file format for DEM simulations and implications for the community of the transition from CPU-based to GPU-based HPC systems. Training was delivered on data visualisation with ParaView, advanced deep learning techniques, and running LAMMPS simulations on a GPU.

It is noted that this technical training encompasses some important cross-cutting topics: accelerated computing (Network Event 4), and developments or applications of AI (Network Events 3 & 4). The embedding of green computing in community workflows entails the linking together of running GPU-enabled codes (Network Event 4) on HPC (Network Event 2), the next generation of which will be predominantly GPU-based for energy efficiency reasons.

In addition to technical training, two significant outputs are under development. Firstly, CCC-ParaSolS began a code development project in January 2026 following a community consultation in 2025. This will result in the open-source MercuryDPM code being able to run on GPUs and heterogenous architectures: capabilities which this DEM code currently lacks. This code development is being done in two stages. Stage 1 entails adding particle capabilities to the OPS embedded domain specific language to create ‘OPS-Particle’; stage 2 will involve integrating OPS-Particle with MercuryDPM. The other ongoing technical project is the development of code benchmarking cases based on silo discharge, which will include the three codes prioritised by CCC-ParaSolS: LAMMPS, MercuryDPM and YADE.

3. Research Implications and Impact

The impact of the training identified in Section 2 is the number of community members who have benefited from it. To extend the benefit beyond the 30–40 people in attendance at each Network Event, the training materials are all online (see Section 4). The training delivered on the adoption of open-source codes for particulate solids simulations and their deployment on HPC and GPUs are intended to overcome one element of the Grand Challenges facing our community: the particulate solids simulation community has historically favoured commercial codes run on workstations, limiting the scale of the problem that can be simulated and not taking advantage of the UK’s Digital Research Infrastructure (DRI).

The synergy with the UK's current Industrial Strategy is clear. The IS-8 sectors with the highest potential will be supported, several of which involve particulate solids, most obviously Advanced Manufacturing and Clean Energy Industries. Simulations of particulate solids — the subject of CCC-ParaSolS — will be highly impactful if expanded in usage within these sectors from 2026 levels.

4. Up to 5 research outputs that create an impact story for your community

The main research output from CCC-ParaSolS is a repository of training materials and learning resources, to benefit researchers starting to use DEM, learning a new open-source code, aiming to get started with AI/ML, or wishing to get started with HPC or GPUs: ccc-parasols.ed.ac.uk/resources/tutorials & ccc-parasols.ed.ac.uk/resources/learning_materials. The tutorials are also being added to a Zenodo Community: https://zenodo.org/communities/parasols/

While community members are doing highly impactful research, it is too early to attribute this to CCC-ParaSolS. The two technical outputs described in Section 2 (OPS-Particle and its integration with MercuryDPM, and the code benchmarking cases based on silo discharge) are still under development.

5. Workshops and new opportunities*

Following the programme of four hybrid Network Events, we are organising a series of webinars on practical issues related to DEM, pitched beyond the basic level. Example topics for these webinars include:

- Approaches to pressure control
- Dealing with very wide particle size distributions
- Treatment of periodic boundary conditions in different codes
- Calibration of rolling resistance models
- Fluid coupling
- Code validation
- Bridging from small to large scales
- Modifying DEM codes
- Advanced visualisation with ParaView

These webinars will be advertised via the Discourse forum, LinkedIn and on the project website.

6. Issues and problems*

Clarity about funding to enable these Collaborative Computational Community scoping projects to become full Collaborative Computational Projects after December 2026 would be welcome.

CCP-DCM for the Period 01/10/25 to 31/03/26

CCP Data-centric Computational Mechanics

Prof. David Ham (CCP-DCM Chair)

1. Background

No changes to previous.

2. Outputs

Accelerated computing developments

GPU capability has been identified in our roadmap as a critical community requirement. The 2026.04 release of Firedrake includes GPU offload capability. This enables assembled linear systems to be copied to the GPU and solved there. Similar functionality is in development for FEniCS at https://github.com/FEniCS/dolfinx-gpu-solvers/. GPU functionality will be critical in enabling this community to fully exploit the Digital Research Infrastructure of the future.

Firedrake has established a collaboration with the developers of xDSL, a Python compiler toolkit which is part of the broader MLIR compiler ecosystem employed by the ML/AI community. This promises to enable operator assembly on GPUs, which will enable a much wider range of use cases to benefit from accelerated computing.

Software releases

- Firedrake released version 2025.10 in October 2025 and version 2026.04 in April 2026.
- FEniCS released version 0.10.0 in October 2025 and will release version 0.11.0 by June 2026.

Regular software releases are critical to in supporting our community by providing stable yet updated computational platforms for their research.

Training delivered

- A three-day long Firedrake training event was delivered in Oxford 18-20 March 2026. 48 registered attendees and 8 local MSc/PhD students studied both the basics of solving stationery and time-dependent problems, as well as various advanced topics like geometric multigrid and p-multigrid solvers, high-order mesh generation and adaptive mesh refinement with Netgen, nonlinear problems, mixed formulations and block preconditioners, eigenvalue problems, and adjoints. Attendees came from national academic institutions (Imperial College London, the University of Cambridge, the University of Exeter, University College London, the University of Bristol, the University of Sussex, University of Bath, University of Leicester), international academic institutions (Scuola Normale Superiore di Pisa, University of Coimbra, University of Padova, Eötvös Loránd University, Charles University, University of Limerick, University of Lisboa, University of Galway), and national PSROs (UK Atomic Energy Authority, Science and Technology Facilities Council, British Antarctic Survey).
- A hackathon on the subject of weak 4DVar data assimilation was held at RAL 8-10 April 2026 and led by CoSeC Fellow Jemima Tabaert. Around 20 participants from UK and overseas and from academia, PSREs and industry worked on foundational technology for high performance digital twins. Outputs included the differentiation of the Gusto atmospheric modelling toolkit, the extension of Firedrake's data assimilation

capabilities to encompass field measurements in addition to point data, and work on preconditioning strategies for data assimilation.

- OSSFE 10-12 March 2026, Munich: Invited FEniCS tutorial at nuclear fusion software conference. FEniCS is the basis for FESTIM, an open-source package for modelling tritium transport in nuclear reactors. At OSSFE, we delivered an introductory tutorial to FEniCS for the general audience, and a plenary talk including our latest GPU work. OSSFE had 125 attendees, including participants from national labs (UKAEA, CEA, Oak Ridge) and industry (Proxima Fusion, General Atomics, Tokamak Energy).

3. Research Implications and Impact

Fusion energy research

A highlight of the CCP-DCM community is the extent to which this software now underpins research into fusion power generation, a priority identified in the industrial strategy. Firedrake is directly employed by institutions such as UKAEA and their partners Los Alamos National Laboratory in studies such as https://doi.org/10.5802/smai-jcm.131 on and https://doi.org/10.1088/1741-4326/adf3cc to model plasma dynamics in fusion reactors. Meanwhile the FEniCS-based FESTIM (https://doi.org/10.1016/j.ijhydene.2026.153987) is widely employed to study hydrogen transport in fusion reactors.

4. Up to 5 research outputs that create an impact story for your community

- A paper on the DefElement encyclopaedia of finite elements https://doi.org/10.1007/s44207-026-00011-0. This documents what has become a canonical resource for the entire finite element community, far beyond Firedrake + FEniCS.
- Work with UKAEA has revealed that the main equation solved to understand tokamak fusion reactors has multiple solutions: https://doi.org/10.1088/1741-4326/adf3cc .
- Structure-preserving discretisation's in time https://doi.org/10.1137/25M1756673 . A new technique that allows for preservation of laws like conservation laws and dissipation inequalities. For example, with this we devise the first Eulerian discretisation of the compressible Navier--Stokes equations that preserves mass-, momentum-, and energy-conservation, while also provably dissipating entropy.
- Expressing general constitutive models in FEniCSx using external operators and algorithmic automatic differentiation https://doi.org/10.46298/jtcam.14449 In this article, we describe a methodology and software framework for FEniCSx/DOLFINx that enables the expression of constitutive models in nearly any general programming language.
- FESTIM v2.0: Upgraded framework for multi-species hydrogen transport and enhanced performance https://doi.org/10.1016/j.ijhydene.2026.153987 Nuclear material modelling for fusion reactors.

5. Workshops and new opportunities*

- Firedrake/PETSc Users and Developers Meeting 1-5 June https://www.firedrakeproject.org/firedrake_26.html

- FEniCS meeting 17-19 June https://fenicsproject.org/fenics-2026/
- FEniCS online tutorial/conference (in planning, joint with Simula, Norway) - Autumn 2026.

6. Issues and problems*

None.

CCP-TEPP for the Period 01/10/25 to 31/03/26

Towards a Collaborative Computational Project in Theoretical and Experimental Particle Physics

Dr. Ed Bennett (CCP-TEPP Chair)

1. Background

No changes to previous

2. Outputs

Comms
The project now has a website at https://ccp-tepp.github.io, and an announcement mailing list as CCP-TEPP-ANNOUNCE JISCMail.

Roadmap
Following last year's workshops, our full *Roadmap for Software for UK Particle Physics* is now finalised and available on the CCP-TEPP website.

Docathon
An issue identified as common across the TEPP community as part of our road mapping process was that particle physics software would benefit from improved documentation—including both user-facing and developer-facing documentation. To support improvement in this space, we organised a Docathon at the University of Warwick in March 2026. Teams from experiment and theory met for 2.5 days; following an introductory talk from Andrew Lister of CoSeC, the teams worked to implement documentation improvements in widely-used community software. There was a particular focus on automated documentation with Doxygen and similar tooling. Pull requests to introduce these changes upstream are in preparation. A more detailed report on this event is in preparation and will be shared on the CCP-TEPP website.

Hadrons hackathon
Within the lattice subcommunity, issues identified in our road mapping process included enabling measurement codes to transition to GPUs and improving maintainability; one route suggested to this was supporting groups in migrating to the Hadrons library, which is actively developed in the UK and has first-class GPU support. To this end, we organised a Hackathon at the University of Edinburgh in April 2026. This brought together researchers and RSEs from three

major lattice collaborations with a footprint in the UK, to work on developing a reimplementation of their current workflow based on Hadrons, and testing this against their current implementations. All collaborations reported making progress towards these goals; a more detailed report is in preparation and will be shared on the CCP-TEPP website.

Technical work on Grid code
Grid is a major community code in the lattice subcommunity and is developed and maintained within the UK. As part of the process of encouraging more cross-community and cross-software-suite working, a step identified as part of the road mapping process was improving compatibility of lattice software suites with community standards defined by the International Lattice Data Grid (ILDG). To this end, Gaurav Ray in Swansea has focused on updating the implementation of the ILDG standard in Grid to output standards-compliant binary files, and additionally to extend it to the most recent version of the specification reducing the storage requirement for many collaborations making use of the code. This is now in testing and will be pull requested to the upstream code over the summer.

Technical work on Geant4 code
Geant4 is a major community code in the experiment subcommunity, with significant use outside TEPP in the medical, space, and nuclear engineering domains. The experiment road mapping process identified improving API documentation and testing coverage of codes as a specific need in widely used community codes. Heather Ratcliffe at Warwick has thus focused on providing the foundations for building Doxygen API documentation and Google Test based unit tests within Geant4, translating existing code comments into full interface docstrings with inputs, outputs and pre/post conditions. The foundation work has been up streamed to Geant4 recently, with work continuing to expand the documentation coverage in key areas and identifying priority areas for adding unit tests.

3. Research Implications and Impact

Geant4 is a widely used open-source software toolkit for simulating how radiation interacts with matter, and a critical simulation component in the increasingly high-throughput and GPU-based processing pipelines needed to address TEPP Grand Challenges. Through expanded documentation and unit tests, the outputs encode physics behaviour and computational guarantees in the software itself, providing a robust foundation for development and validation of the GPU-enabled components required to meet future demands. This also benefits a broader range of UK research and industry outside of particle physics, including medical imaging and radiotherapy, space science, fusion and nuclear energy, and radiation protection that rely on Geant4 for radiation transport simulation, providing clearer documentation and enhanced reliability.

We are continuing to build bridges with supranational partners pursuing similar goals, including the HEP Software Foundation and EuroLFT.

4. Up to 5 research outputs that create an impact story for your community

- CCP-TEPP, Roadmap for Software for UK Particle Physics, https://ccp-tepp.github.io/documents
- Kourlitis, et al. Optimizing the ATLAS Geant4 detector simulation software, *J.Phys.Conf.Ser.* 3206 (2026) 1, 012035
- FPF Collaboration, The forward physics facility: Physics opportunities and conceptual design, *Nucl.Phys.B* 1026 (2026) 117398

5. Workshops and new opportunities*

- CCP-TEPP Summer School, Swansea University, June 29–July 3
- Road mapping workshops, Autumn 2026, dates tbc

6. Issues and problems*

Cuts in STFC funding for particle physics are preoccupying many discussions currently. Workshop participation is lower than we would have hoped due to some potential participants who we had identified during the road mapping workshop having left the field; there is severe risk of a brain drain that appears to be particularly severe for those who have technical and computational expertise.

Delays in appointing CoSeC personnel to support, particularly on experimental side.

CCP-UKNR for the Period 01/11/25 to 1/6/2026

CCP UK Numerical Relativity

Prof. Eugene Lim (CCP-UKNR Chair)

1. Background

No change to previous.

2. Highlights for the current reporting period

a) We held our **UKNR-CCP 2025 Annual Conference** in **Birmingham** from **Dec 15-16**. (https://www.uknumericalrelativity.org/meetings-conferences/uknr-2025-in-birmingham). This annual event (that began before we joined the CCP) brought together more than 30 members of our community to share scientific and technical results with each other. We also had several international guests, including Tom Giblin from Kenyon College/Case Western University and Mary Gerhardinger from Rochester University. In addition, we held a community-wide discussion of the Grand Challenge Roadmap and our activities for the coming year.

b) In collaboration with the international astrophysics' community, UKNR-CCP is funding and jointly organizing a **AI in Numerical Relativity Zero Day Workshop** in Southampton as part of the annual CocoNut Meeting on Relativistic Astrophysics.

c) Led by Technical Lead **Miren Radia**, the **UKNR-CCP Code readiness Benchmarking exercise** is nearly completion. All required runs have been completed (with many thanks to DiRAC for providing discretion compute from COSMA8 and Tursa), and we are in the process of writing the final report which will (a) provide benchmark reports on UKNR-CCP community codes **ETK Cactus, ETK Cactus-X, GRTeclyn, ExaGRyPE2, GRChombo, MHDuet,** and **BAM** for both CPUs and (where applicable) GPUs. We have also increased the scope of the project which we funded by obtaining a rapid-turnaround **SHAREing** grant (£22,641). Our final product, to be published and open sourced, will be a full set of code "readiness" benchmarks which will include code efficiency and ease of setup, and supplemented by working exemplars of code and parameter files.

d) Our **UKNR-CCP/CoSeC Collaborative project** kicked off officially in Jan 2026. The project involved the development and deployment of *Apparent Horizon Finder (AHF)* in two UK-led GPU-ready codes, **GRTeclyn** and **ExaGRyPE2**. The AHF is a key code functionality which **identifies the existence and extend of black holes** (i.e. "the event horizon") in numerical relativity codes. As the two codes have very different underlying finite difference engines, we split this collaboration into two teams. The first team ("Team GRTeclyn"), consisting of CoSeC member **Adam Greenbank** and UKNR-CCP members **Sam Brady, Katy Clough** and **Eugene Lim**, works on the AHF on GRTeclyn using the particle functionality of the underlying AMReX solver to dynamically trace out the apparent (black hole) horizon. The second team ("Team ExaGRyPE2"), consisting of CoSeC members **Wendi Liu** and **Omar Mahfoze**, and UKNR-CCP members **Zhang Han**, **Tobias Weinzierl** and **Baojiu Li**, uses grid interpolation across different refinement levels. Team GRTeclyn has implemented a prototype pseudo-transient continuation (PTC) solver and is progressing towards the full solution by adding derivatives functionality on top of the underlying grid structure. Team ExaGRyPE2 has established the core C++ and Python class modules required to support the extraction of the underlying grid variables. Instead of a PTC, full solution of the AHF will be obtained using a shooting algorithm instead. Both projects are on schedule and we expect them to be completed and rolled out to users by the end of the year.

3. Research Implications and Impact

a) The cross-cutting work of the UKNR-CCP/CoSeC collaborative project is benefiting both communities. On the UKNR-CCP side, we are learning new advanced mathematical techniques in finding solutions to elliptic PDEs (e.g. PTC and particle-based

techniques), while the CoSeC side is developing an “in-house” working basis of NR in addition to being afforded a “real world test case” of applied mathematics. This collaboration is in line with our community Grand Challenge of maintaining international leadership in NR, and “doing more with less”.

b) The extended scope of our community code Benchmarking exercise means that we intend to publish our benchmarking results and identify the “GPU-readiness” of each code. As these codes are used internationally, this will have impact across the international physics community.

c) The growing interest in the UKNR-CCP community to explore the use of AI in NR has led to UKNR-CCP co-organising and funding the AI in NR Zero Day workshop. As the workshop is attached to an international community of relativistic astrophysics, we expect a wide international participation. By bringing together all the pioneers of AI techniques in NR, we hope to accelerate this research direction, which is part of our community Grand Challenge.

4. Up to 5 research outputs that create an impact story for your community

a) **Katy Clough** and **Eugene Lim**’s innovative use of NR to probe the origins of the Big Bang was featured as a cover story for the 21 February 2026 print issue of the *New Scientist* magazine (https://www.newscientist.com/issue/3583/), with 360k weekly print and 75k online subscriptions. By using NR, Clough and Lim have solved hitherto unsolvable strong gravity equations at the beginning of the Big Bang, allowing scientists to glimpse into the physics of the universe before it. As part of this issue, Katy Clough was interviewed by New Scientist on YouTube (https://www.youtube.com/watch?v=Zr9Ox-msEFc) (117k views as of May 2026).

b) UKNR-CCP researchers from Cardiff and Southampton led by **Mark Hannam** and **Jonathan Thompson** completed the first NR simulations of highly precessing black hole binaries with mass ratio of 20 – arguably the most challenging binary configurations ever attempted by scientists. This massive simulation requires over 10M CPU/hrs. They demonstrated that presently used semi-analytic signal models at this high mass ratio (and above) are woefully inaccurate, hence identifying a major challenge facing the field as the next generation GW detectors will probe mass ratios of over 1000. This is presently in preprint stage (https://arxiv.org/abs/2603.26521).

c) **Ulrich Sperhake** and his research group at Cambridge produced the longest and most stable NR simulations of the so-called "black hole mimickers" : objects that behave almost but not quite like black holes. These are important "test cases" for scientists to probe new physics beyond Einstein's gravity. This simulation is especially challenging – indeed much more challenging than black hole simulations as it involves an additional mass scale. This work is published in *Physical Review Letters*, *PRL 135 (2025) 13 131402*.
d) Community members from Southampton, led by **Charlie Hoy** has published a key paper in *Nature Astronomy (Nat. Astronomy 9 1256-1267)* on the accuracy of gravitational wave analysis, by comparing it with high precision NR simulations and standard waveforms models use in GW detection experiments. In particular, they introduced an efficient technique which uses 30% less computational resources to obtain a more precise estimate of black hole merger parameters from data.
e) Community members **Katy Clough** and **Pedro Ferreira** are part of an international collaboration with MIT which produced the first meaningful physical bounds on dark matter using GW data, by numerically computing how GW signatures are modulated by the presence of dark matter near black holes. This work was published in *Physical Review Letters*, *PRL 136 191402* and was highlighted in *Space.com* (https://www.space.com/astronomy/dark-universe/we-still-cant-see-dark-matter-but-what-if-we-can-hear-it) and the *Daily Mail* (~700k circulation) (https://www.dailymail.com/sciencetech/article-15826813/Dark-matter-detected-seven-YEARS.html).

5. Workshops and new opportunities*

a) UKNR-CCP Summer Workshop in (Oxford, 8-10 June)
b) UKNR-CCP AI Applications in NR Zero Day Workshop (Southampton, 8 Sept) – this workshop would be of interest to other CCPs who are exploring the use of AI to solve PDEs (e.g. the CFD community).
c) UKNR-CCP 2026 Annual Meeting (Late Autumn, location TBA).

6. Issues and problems*

None.

CCP-AHC for the Period 01/10/25 to 31/03/26

Towards a Collaborative Computational Project (serving Arts, Humanities, and Culture researchers

Dr. Eamonn Bell (CCP-AHC Chair)

1. Background

CCP-AHC (www.ccpahc.ac.uk) focuses on DRI and software that support computationally intensive research and innovation in the arts, humanities, and culture (AHC) fields. This

research is typically funded by in the UK by UKRI's Arts and Humanities Research Council (AHRC). Our scope includes any code, pipelines, or workflows developed by the community that is running or has the potential to run on UK-funded HPC and advanced computing resource, including those targeting GPUs and other novel accelerators.

Earlier efforts to gather community requirements targeting AHRC-facing researchers offer some insights into HPC and cloud computing usage to date, where 38% of survey respondents used or were moving to "HPC/Cloud" in 2021. Our aim is to increase this proportion by curating a portfolio of codes, pipelines, and workflows that represent community needs and ambitions for computationally intensive AHC research.

We also recognise the vital role of data in driving adoption of digital methods, so we work with AHR funded data services and other activities to raise the awareness of existing large-scale compute provision and promote wider UK DRI engagement activities. These include the FAIR data infrastructures within the AHRC's portfolio of DRI projects, the Infrastructure for Digital Arts and Humanities (iDAH), the national DRI skills hubs, and ongoing Network+ activities in federated and sustainable computing.

We have continued to identify those software projects with the potential for development through engagement with RSE and computational science resource within CCP-AHC and CoSeC during the scoping project and over the longer-term future of the project and related initiatives.

We do this through a combination of responsive open calls for research software submissions, desk research, and community engagement exercises. We are in the process of onboarding the first wave of about c. 15 software projects by including inviting them to participate in the CCP-AHC technical working group, which meets biweekly.

Work is co-ordinated and meeting minutes are now publicly posted on the CCP-AHC GitHub organisation (http://www.github.com/ccpahc), which serves as the open forum to co-ordinate technical effort in the community. We will refine this onboarding and governance approach based on the experience of the first cohort and further widen the community beyond this initial set before the end of the scoping period.

2. Outputs

Work is underway to increase the FAIRness of community codes. This is being led by RSEs at Durham who propose the inclusion of Codemeta (https://codemeta.github.io/) metadata files as pull requests against community-owned repositories. This will ultimately increase the discoverability of CCP-AHC software, and lead to the production of a software directory (cf. https://tools.clariah.nl), supporting metadata harvesting by other repository initiatives such as the AHRC-funded Data/Culture portal and the SSH Open Marketplace (https://marketplace.sshopencloud.eu/)

In April and May 2026 community members attended a two-part online training on community code review delivered by members of the ADHO DHTech SIG, led by Julia Damerow (RSE,

Arizona State University). This covered the basics of code review, a useful overview of the features of collaborative version control software that support code review, and an overview of tools used to improve code quality and reviews (e.g. commit hooks, linters, CI/CD). A follow-up meeting was held to elicit requirements from code owners considering the training.

We have grown the JISCMail mailing lists for CCP-AHC-ANNOUNCE (announcements and news) and CCP-AHC-DISCUSS (community discussion) to 133 and 85 subscribers (up from 119 and 79, respectively). Monthly online CCP-AHC Community Forums continue, with guest presentations from the AHRC-funded Data/Culture project and several NFCS Network+ projects, and a special introduction to the EOSC EU Node services since January 2026.

Given the widespread interest in and adoption of AI methods within the field, we are building a network with infrastructures that have the potential to drive engagement with and widen access to existing DRI that supports these methods and the preferred access modalities for less technical users. We note the recent announcement of funding for the UK-Ireland Digital Humanities
Association until 2028 (by the DRI programme) and the UKRI-funded Mapping the Humanities and AI project at the School of Advanced Studies, University of London (https://blog.humanities.org.uk/2026/02/25/in-development-mapping-humanities-and-ai/).

As an international example, the useGalaxy.eu platform supports experimental access to openweights large language models (LLMs) and multimodal models hosted at the University of Freiburg. 10 community members participated in the global, asynchronous Galaxy Training Academy 2026 (https://training.galaxyproject.org/training-material/events/2026-05-18-galaxy-academy.html), working on the Digital Humanities track.

We expect their experiences to inform requirements for technical development work increasing the nascent support of the Galaxy platform for arts and humanities (and social science) research. This will be co-ordinated by CCP-AHC presence at the Galaxy Community Conference (GCC) 2026 (June 2026) and the CoFest Hackathon.

The adoption of Galaxy also opens opportunities for increased cross-council working with (e.g.) members of the BioFAIR infrastructure and the ongoing development of a UK-based server instance. Some AHC capacity could be backed by a small reservation of classical HPC resource within the future UK DRI compute ecosystem, using the Pulsar middleware.

Based on community requirements elicitation events held in late 2025, CCP-AHC members have contributed to the draft report “Inclusive Futures for the National Federation of Digital Research Infrastructures” (forthcoming) and the interim “Federated Digital Research Infrastructures (DRI) for the Arts and Humanities Communities” (https://zenodo.org/records/18350953). CCP-AHC now sends a delegate to regular meetings with the heads of other AHC data services in anticipation of increased federation of the AHRC-funded DRI components.

3. Research Implications and Impact

Work to prioritise projects in the application of AI to arts, humanities, and cultural datasets continues. These include automatic speech recognition, optical character recognition, handwritten text recognition, document layout analysis, visual question answering, and zero-shot text and image classification.

We have successfully experimented with the deployment of one GPU-intensive software to the EOSC
EU Node container platform, illustrating the use of the tool to index a collection of images hosted by Durham University Library and Collections using the open IIIF image interoperability standard. This increases the availability of multimodal visual AI to researchers and cultural heritage collections.

Work is underway to contribute this documentation back to the upstream project and to identify similar "quick win" illustrations of the benefits of a single point-of-contact for shared compute. We are also keeping a watching brief on the adoption of LLMs to support programming (especially "agentic coding"), to support the rapid development of prototypes by non-programmers.

Together these efforts contribute to the CCP-AHC Grand Challenge of widening access to AI for arts, humanities, and culture research.

4. Up to 5 research outputs that create an impact story for your community

Finnigan, Samantha. 'Archaeological Rendering at 2,600 Models per Hour: HPC for Digital Heritage Collections'. CCP-AHC Blog, 27 February 2026. https://www.ccpahc.ac.uk/blog/2026/02/27/archaeological-rendering-at-2600-models-per-hourhttps://www.ccpahc.ac.uk/blog/2026/02/27/archaeological-rendering-at-2600-models-per-hour-hpc-for-digital-heritage-collections/hpc-for-digital-heritage-collections/.

Bell, Eamonn. 'Developing Actionable Workflows for the Social Sciences and Humanities with Galaxy'. CCP-AHC Blog, 29 April 2026. https://www.ccpahc.ac.uk/blog/2026/04/29/developinghttps://www.ccpahc.ac.uk/blog/2026/04/29/developing-actionable-workflows-for-the-social-sciences-and-humanities-with-galaxy/actionable-workflows-for-the-social-sciences-and-humanities-with-galaxy/.

5. Workshops and new opportunities*

- CCP-AHC Town Hall 2026 – 17th September 2026, STFC Rutherford Appleton Laboratory (Harwell, Oxfordshire)
- Directly preceded by CCP-AHC training activity – (afternoon) 16th September 2026, STFC Rutherford Appleton Laboratory (Harwell, Oxfordshire)

6. Issues and problems*

We await details of the funding instrument that will support the continuation of successful CCP scoping activities.

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