CoSeC

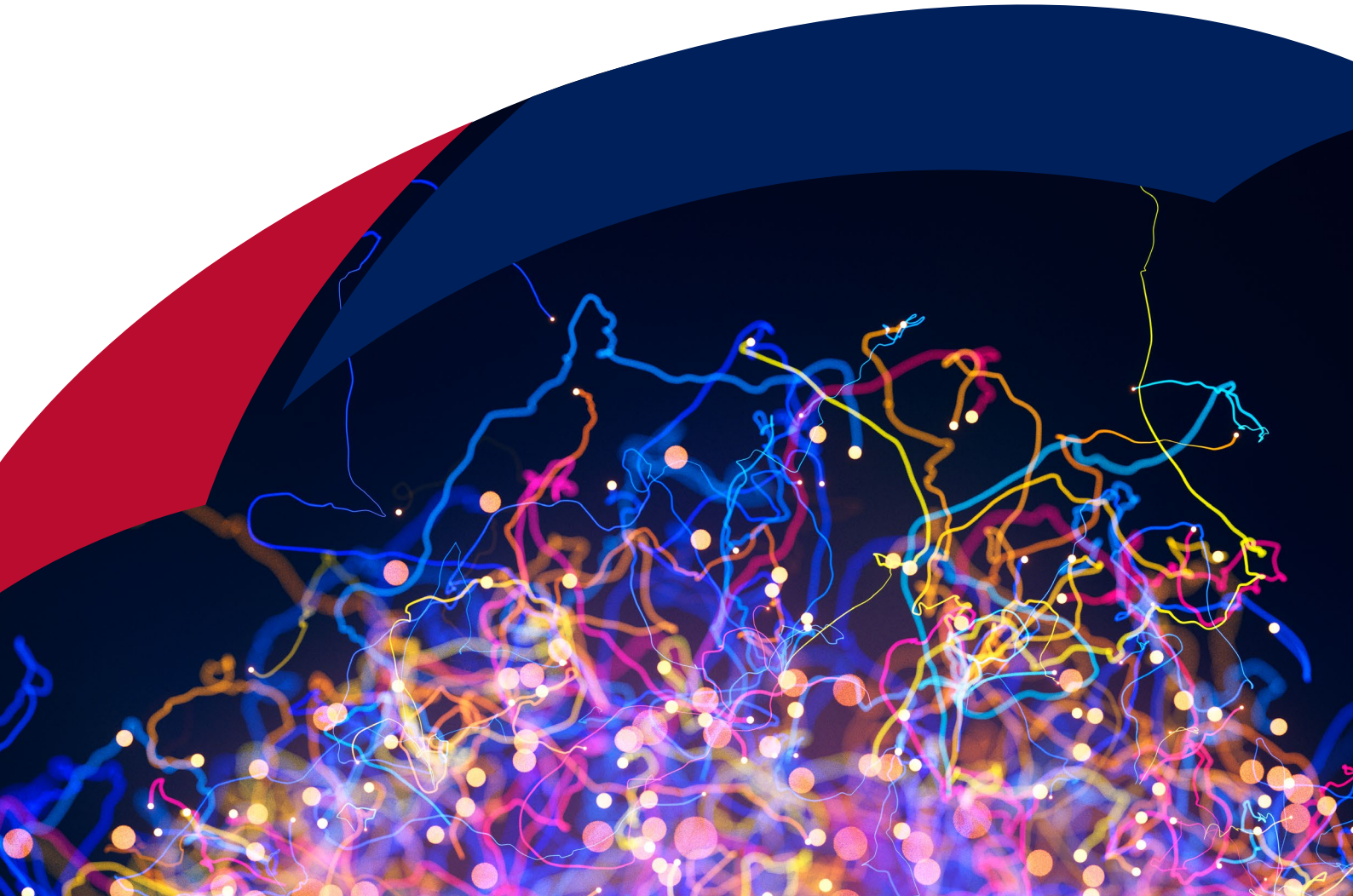
Computational Science Centre
for Research Communities

UKRI Science and Technology Facilities Council

Scientific Computing

2025-26 Annual Report

April 2026



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Introduction

The Computational Science Centre for Research Communities (CoSeC) is a UKRI Centre that supports collaborative computational research across the UK by developing and maintaining research software, coordinating computational communities, and the enabling effective use of national digital research infrastructure.

Operated by UKRI STFC Scientific Computing, it is comprised of specialist technical teams working with collaborative computational communities known as the CCPs and HEC consortia, as well as a dedicated Programme Office. Its core activities include advancing algorithms and research software, scanning and articulating future technology landscapes and challenges related to domain-specific research. CoSeC also provides training and user support, manages FAIR standards, and promotes sustainable software practices. We are committed to strengthening community networks, and supporting the Research Technical Professional career pathway with a focus on equality, diversity, and inclusion.

This annual report highlights the work of CoSeC over the last financial year. It includes examples through a selection of research case studies and comments from CoSeC's team. The report will outline key metrics and introduce you to initiatives such as the CoSeC Fellowship Programme and our annual awards. You will also read about CoSeC events that have taken place and funding opportunities we are currently delivering.

Read more about CoSeC

cosec.ac.uk

Highlights of the Year

Over the past five decades, organised, domain specific communities have supported and sustained vital research software for the UK. Throughout this time, CoSeC has been a key component of this formula, adapting to meet the changing needs of the research landscape. Over the past year, this evolution has accelerated, with significant changes shaping the future of CoSeC.

The last year has been transformative for us. Following investment from the UKRI Digital Research Infrastructure (DRI) programme in 2024, we are actively delivering a new phase of activity. Some changes are highly visible, such as the launch of our new website at the start of 2025, whilst others are structural, strengthening our engagement with UKRI research communities for the long-term.

The last twelve months have been especially productive, with achievements spanning technical developments delivered alongside our communities and through our own cross cutting work to improve software energy efficiency and make community data more FAIR (Findable, Accessible, Interoperable and Reusable). These activities are guided by CoSeC's strategic priorities: applied AI and machine learning, accelerated computing including GPUs, energy efficient software, and technical training.

Access to the UK's national supercomputing service, ARCHER2, has been essential to our work, enabling optimisation of research software for large-scale challenges. Some of the outputs supported by this resource are described later in the report, and we are grateful to EPSRC for making this possible.

A major highlight of the year was the publication of CoSeC's Grand Challenges. This first cross community convening exercise represents a substantial collective effort and clearly sets out the domain specific challenges across our key research areas. It also demonstrates how these challenges align with the Government's 2025 Industrial Strategy. Our Grand Challenges represent an enormous, concerted effort by all of CoSeC's staff and amazing input from across our communities and will be the basis for the design of our future phases.

Visit the CoSeC website

cosec.ac.uk

Looking to the Future

CoSeC brings together the DRI priorities of multiple UKRI research councils, including BBSRC, EPSRC and MRC, and forms an integral part of the UKRI DRI programme, from which it also reaches into other research domains such as AHRC and STFC. Each of these stakeholders brings a unique element to what CoSeC does and together allow us to support UK research through technical delivery, while also contributing strategically to the DRI agenda. We value our position within UKRI's National Laboratories and are grateful for the opportunity to support the UK research landscape.

Over the next year, CoSeC's transformation will continue to accelerate, guided by stakeholder strategies and oversight from our external advisory board. This work takes place amid changes to the UK DRI landscape, including the transition from ARCHER2 to the Next National Supercomputing Service and the expansion of the AI Research Resource (AIRR). These developments will significantly shape and strengthen the environment in which our communities operate.

The next year will be one of change. Not just for CoSeC, but for all the communities where we work and our colleagues who work within them. Such change brings challenges and must be managed carefully to ensure positive impact. I firmly believe that the high-level visions driving this change are in the right direction for a future where we can plan and create long-term strategies for computational research in a way that has not been possible before.

Record government investment in DRI presents us with a unique opportunity: a coordinated national compute capability, complemented by sovereign AI resources. The question therefore is what this investment will look like in terms of the necessary research software infrastructure that this capability will demand. A critical next step is ensuring that CoSeC's research software infrastructure evolves to match this capability, enabling effective use of new resources and delivery against the Government's strategic national priorities.

Stephen Longshaw

Director of CoSeC

Grand Challenges

In 2025, CoSeC began to explore the Grand Challenges that exist in the domain areas of our communities over the coming decade. The purpose of this exercise was to identify a set of high-level challenges relevant for computational research within the UK and to produce a set of guiding statements that encompass the aims and objectives of UKRI's Digital Research Infrastructure.

The Grand Challenges highlighted the reasons why they are seen as challenges, as well as the processes that we, along with the communities will follow to address them. These range from high-level challenges that stem from key national goals identified in the 2025 Modern Industrial Strategy through to domain-specific drivers that form the long-term plans encapsulated by each community.

While domain-specific, these challenges share common drivers: scale and complexity of data, transition to heterogeneous and exascale computing, integration of AI with physics-based models, the need for validation and trust, and the requirement to make advanced computational capability accessible beyond specialist groups.

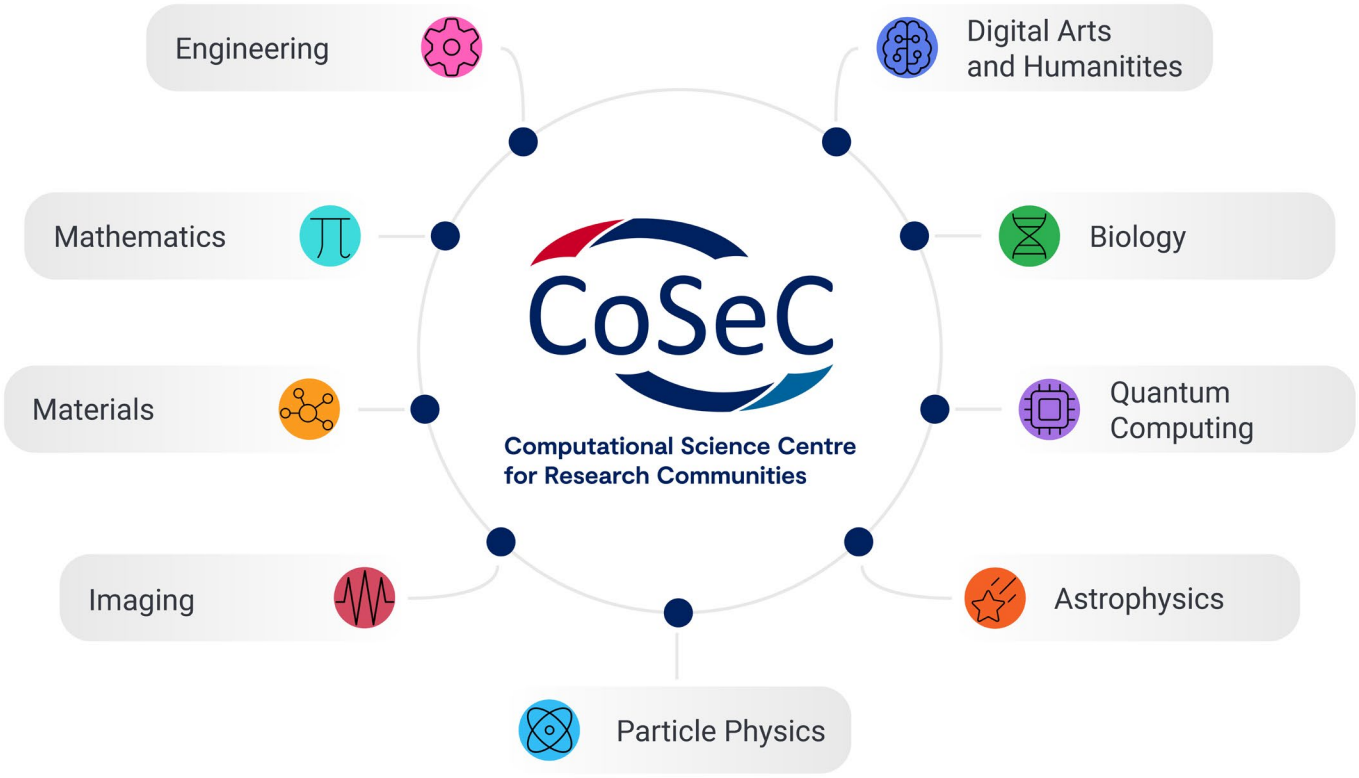
Across the communities, a consistent theme emerges within each of the challenges that relate directly to the goals of UKRI's Digital Research Infrastructure:

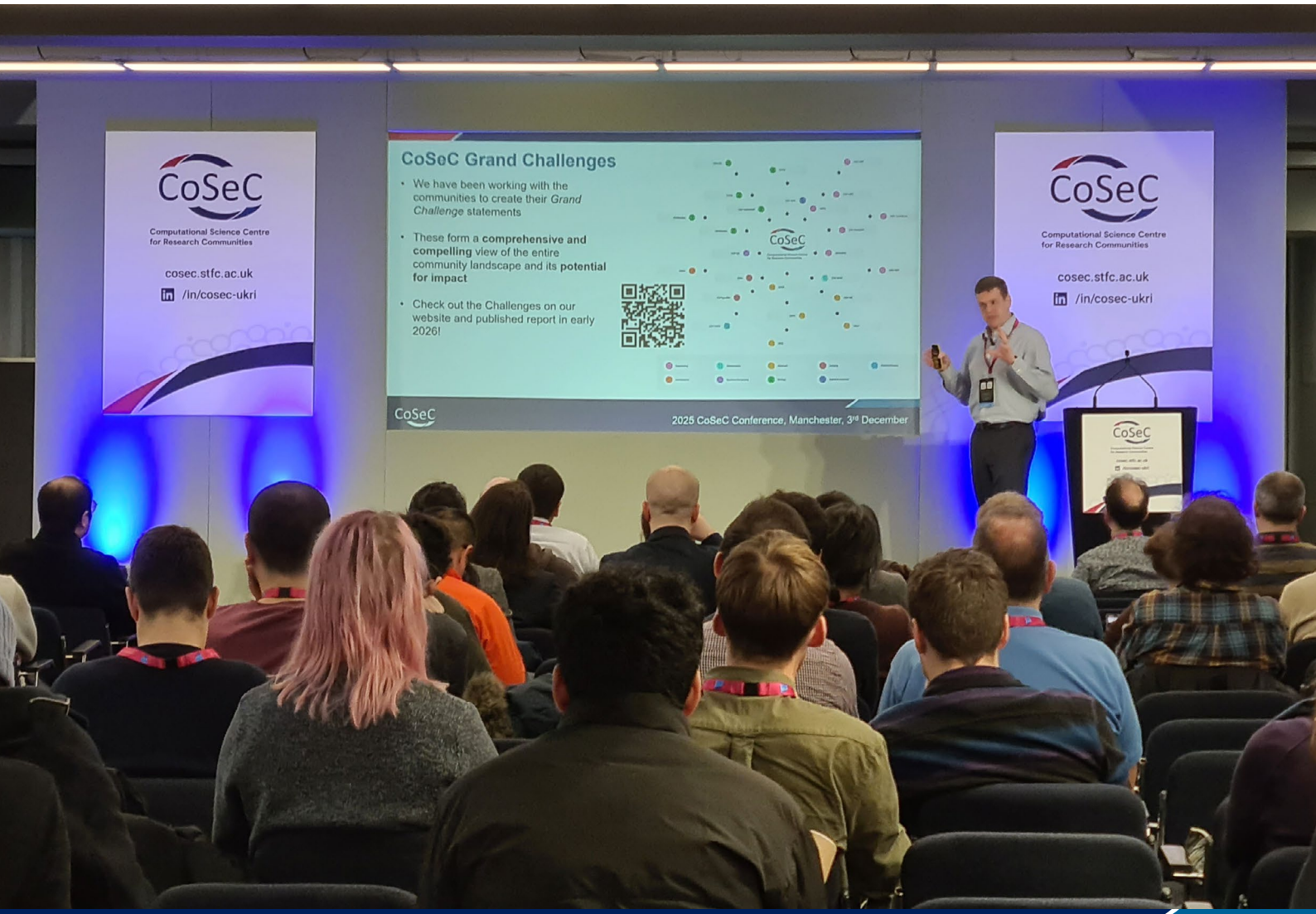
- Scaling to exascale and utilising heterogeneous compute architectures
- Integrating AI and ML into modelling workflows
- Ensuring Findable, Accessible, Interoperable and Reusable (FAIR) high-quality data
- Developing interoperable software ecosystems both across and between communities
- Training diverse communities of researchers, Research Technical Professionals (RTPs) and domain users.

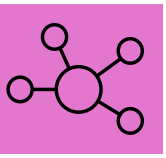
Together with us, the Collaborative Computational Project (CCP) and High-End Computing Consortia (HEC) communities outline a roadmap for UK computational research that underpins national priorities in key areas such as Net Zero, energy security, health, advanced manufacturing, and sovereign capability around digital research infrastructure. There is convergence on a common goal of creating scalable, energy-efficient, AI-integrated computation that is validated, trusted, and accessible, enabling UK research and industry to exploit digital research infrastructure as a strategic national asset.

When grouped into thematic areas, it is possible to gain high-level insight into the common threads that exist amongst them.

Community Landscape







Engineering

Delivering predictive, validated, and computationally scalable multiphysics simulation for use by industry and on national digital infrastructure.
Across engineering communities (particulate solids, turbulence and wind energy, porous media, wave–structure interaction, and nuclear thermal hydraulics), a key challenge is moving from bespoke or workstation-scale modelling to high-fidelity, validated simulation at real-world scale, capable of informing industrial deployment and regulatory decisions. This requires exploiting heterogeneous HPC (GPUs, large-scale systems, and emerging architectures), integrating AI with solvers, and ensuring access to and curation of high-quality data.

Mathematics and Fundamentals

Democratising high-fidelity digital twins beyond elite HPC centres.
The mathematics community (data-driven computational mechanics) identifies that enabling widespread adoption of digital twins across research, engineering, and medicine is key. While digital twins underpin strategic national priority areas, their use remains limited by computational cost and specialist expertise and, importantly, the underlying cross-disciplinary software infrastructure they demand.

Materials

Preparing materials modelling for AI-enabled, quantum-aware, and energy-efficient next-generation computing.
Materials communities (electronic structure, condensed phases, materials chemistry, and Car–Parrinello methods) face a convergence of scientific ambition and computational constraint. The combined challenge is to extend predictive materials modelling across scales and technologies, whilst exploiting AI and quantum computing and managing energy efficiency.

Imaging

Evolving imaging from inspection to quantitative, real-time decision making platforms for use in national priority areas such as healthcare.
Imaging communities (tomographic imaging and synergistic biomedical imaging) identify a combined challenge in transforming CT, MRI, and PET from post-inspection tools into real-time quantitative, high-throughput, multimodal platforms for industry and healthcare.

Biology

Transforming data-intensive structural and molecular biology into integrated, scalable, and trustworthy computational workflows.
Biology communities (cryo-EM, crystallography, volume electron microscopy, and biomolecular simulation) face explosive growth in data volume and methodological complexity. The challenge is to convert this into reliable, interpretable biological insight at scale, while managing storage, compute cost, and skills.

Astrophysics

Sustaining UK leadership in gravitational-wave science through precision, efficiency, and sovereignty.

Numerical relativity faces the dual challenge of increasing mathematical precision to match next-generation gravitational-wave detectors while reducing computational cost and energy use. At the same time, increased reliance on non-UK software infrastructure raises concerns about digital sovereignty with opportunity for organised UK-based communities to make ongoing coherent decisions in the national interest.

Quantum Computing

Embedding quantum computing into trusted, regulated research and industrial workflows.

The quantum computing community's challenge is not hardware alone, but early, meaningful integration of quantum computation into existing HPC workflows in a way that delivers real-world research value.

Particle Physics

Transforming computation to meet an order-of-magnitude increase in data and precision.

Particle physics confronts unprecedented data volumes from next-generation experiments both from within the UK and internationally as well as rising demands for theoretical precision. The Grand Challenge is to re-engineer trusted computational methods and software frameworks to enable real-time data processing, simulation, and analysis at large computational scales.

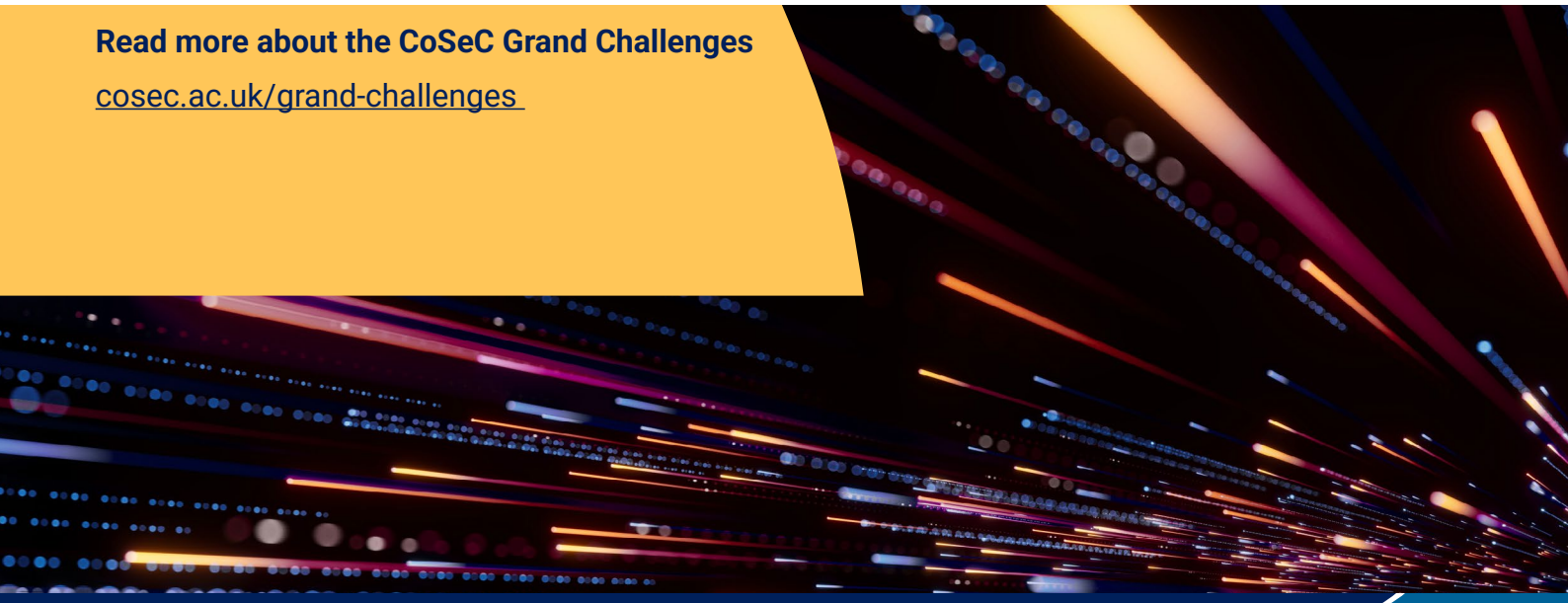
Digital Humanities

Enabling equitable, large-scale AI analysis of cultural heritage and humanities data.

The digital humanities community needs to make trusted AI-enabled analysis of vast cultural datasets accessible to researchers regardless of technical background or institutional resources.

Read more about the CoSeC Grand Challenges

cosec.ac.uk/grand-challenges



ARCHER2 Projects

As part of our strategic partnership with EPSRC, CoSeC is granted access to the UK's national supercomputing service, ARCHER2. This is a key element of how we enable development of research codes for use on national infrastructure that are identified as priorities through the communities we work with. The access allows us to do large-scale testing of codes and debugging on a major HPC platform. It also allows us to identify issues with the service itself related to the software that UK researchers need to run and allows us to help in development of its capability.

Across our diverse domain areas we have used the c01 allocation on ARCHER2 resource allocation to support code development, benchmarking, validation, and large-scale simulations that underpin national computational science capability.

Within CCP-NTH, significant progress has been made on high-fidelity CFD methods and nuclear thermal-hydraulics applications.

- CHAPSim development included verification of new physics modules, billion-cell scalability testing, and detailed benchmarking to identify performance bottlenecks
- RVACS simulations generated high-quality FAIR datasets for model validation, uncertainty quantification, and AI/ML surrogate development, supporting next-generation nuclear reactor safety
- code_saturne development introduced new CDO-based CFD functionalities that will benefit the CCP-NTH, UKTC, and CCPi communities.

Within MCC, the c01-chem team advanced the development and performance of ChemShell and DL-FIND, including QM/MM capability, TD-DFT benchmarking, vibrational spectroscopy workflows, and the integration of ML-accelerated optimisation methods.

Within UKCOMES, c01 time supported functionality testing in DL_POLY_5 and DL_MESO as well as the development of new coarse-grained polarisable water models, contributing to publications and upcoming battery modelling work.

For UKCP, the allocation enabled acceptance testing of CASTEP 26.1.1 in the production environment, ensuring reliability and readiness ahead of academic release.

Within CCPBioSim and cross-cutting CCP-NTH activity, large-scale coupling tests between code_saturne and GROMACS were performed on up to 1,024 nodes. This included addressing MPMD and scaling challenges and supporting development of parallel HDF5 implementations for image-based modelling.

Overall, the c01 allocation has facilitated major advancements in software capability, performance benchmarking, large-scale scientific simulations, and cross-community tool development, strengthening UK HPC scientific infrastructure across multiple CCPs and consortia.

Cross-Cutting Projects

As part of the funding, CoSeC receives from the UKRI DRI, we have been successful in enabling two cross-cutting projects to investigate topics relevant to the work of CoSeC and its communities.

The first is a project on **"Energy Efficient Computing"** led by STFC Software Engineer Jess Huntley and CCP-DCM Project Lead Dr Hussam Al Daas, who are working with CCP communities to identify common challenges related to energy efficient computing and develop follow-up projects to determine and publicise best practice.

Read more about energy efficient computing

cosec.ac.uk/what-is-cosec/cross-cutting-projects/energy-efficient-computing/

Without information on energy efficiency, developers and users are unable to make informed choices about the way they write or use software. Current understanding is limited, and whilst some communities have started developing guidance on energy efficiency, for instance measuring and reducing the carbon footprint of fMRI preprocessing, this is often application specific and time consuming for researchers. This cross-cutting project aims to generalise existing knowledge of sustainable computing and address common challenges across disciplines. As well as building knowledge, this project will also work to build a community across CCPs to embed sustainable computing practices.

Phase 1 and 2 of this project included a workshop organised by CoSeC to better understand the current landscape in terms of energy-efficient computing across all CCPs and start conversations around making energy-efficient choices. The outcomes of that workshop are now being disseminated as the project moves into phase 3, with further information to be made available later in 2026.

Read more about measuring and reducing the carbon footprint of fMRI preprocessing

pubmed.ncbi.nlm.nih.gov/39185668/

The second project funded by CoSeC is the creation and development of the **"CoSeC Catalogue"**.

Research outputs, such as software codes, projects, test cases, publications, data and events are often either not shared at all, or all shared in different places without any links in place to connect them. For example, software codes might be shared via GitHub, data via universities' institutional repositories or Zenodo, events via the websites of individual projects, publications via universities' institutional repositories and so on.
The potential impact of cataloguing these research outputs in one place, so that they are FAIR (Findable, Accessible, Interoperable and Reusable) is high. The result of the application of FAIR attributes is well known and what all data, whether that data is experimental, simulated, or in the form of research outputs, should aim to adhere to.

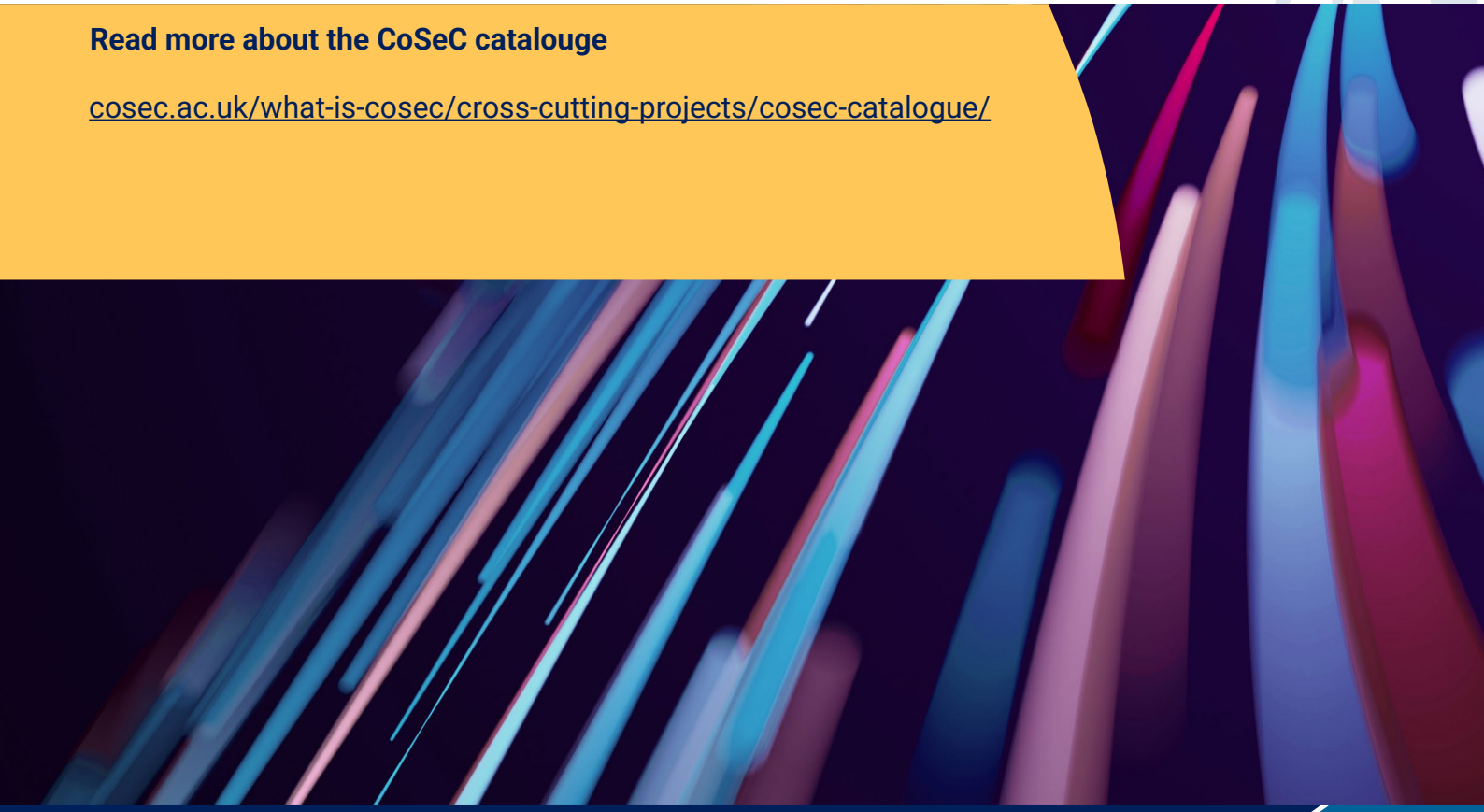
Consequently, CCP-WSI have developed a successful catalogue of research outputs tailored to the field of Wave Structure Interactions and CCP-NTH are committed to doing the same for their scientific domain.

Following on from CAT-WSI, and a catalogue for CCP-NTH, a high-level CoSeC Catalogue is now being developed. This will provide a central location for all the individual CCP catalogues but additionally, the ability to conduct a cross-search over the various domains. The CoSeC Catalogue, therefore, can be thought of as a collection of domain-specific catalogues together with an integrated search across all of them. The main intention of the CoSeC Catalogue is to highlight research outputs, however, the potential impact goes further, including the application of FAIR principles, encouraging collaboration, and making the impact of CoSeC more identifiable and quantifiable.

This project is now in the final stages of development and will be ready to go live this year.

Read more about the CoSeC catalouge

cosec.ac.uk/what-is-cosec/cross-cutting-projects/cosec-catalogue/




Resource Types
Data
Publications
Software
Solvers
Test Cases
Services
All Resources
Grand Challenges
Engineering
Mathematics
Materials
Imaging
Biology
Astrophysics
Quantum Computing
Particle Physics
Digital Humanities
Communities
CCP-WSI
CCP-NTH
CCPi
CCP-EM
CCP5
CCP4
CCP-QC
CCPSyneRBI
HECBioSim
CCPBioSim
CCP-NC
CCPN
CCC-ParaSolS
UKTC
CCP-AHC

Events

6th Manchester Multiscale Conference, March 2025

The 6th Manchester Multiscale Conference (31 March 2025 to 2 April 2025, attended by 102) brought together researchers working on multiscale modelling across electronic, atomistic, and mesoscopic levels. This was followed by several industry seminars highlighting the role of molecular simulation in pharmaceutical research, including talks from AstraZeneca (30 April 2025), Queen's University Belfast (28 May 2025), and Sanofi (11 June 2025).

CCP-EM Symposium & BCI User Meeting, April 2025

The eleventh annual CCP-EM Spring Symposium was held jointly with the BCI User Meeting from 23-25 April 2025. The event ran in a hybrid format, with 1045 total registrations, 36% of which were in person (375) and 67% virtual (630). There were over >2897 hours total watch time, with a mean time in sessions of 4 hours, 44 minutes. Lecture recordings for the majority of speakers are available on the CCP-EM YouTube channel.

The conference was attended by delegates from a variety of career stages. Thanks to the support of sponsors, CCP-EM were able to fund 32 bursaries covering in-person registration fees and accommodation.

CCP-EM also recently published a review of the *Symposium in Acta Crystallographica Section D,* 'Ten years of the CCP-EM Spring Symposium', written by CCP-EM Administrator Lauren Giles and Project Lead Tom Burnley.

Read more about the workshop and the talks involved

tinyurl.com/4xz6p842

CCPi Workshop, April 2025

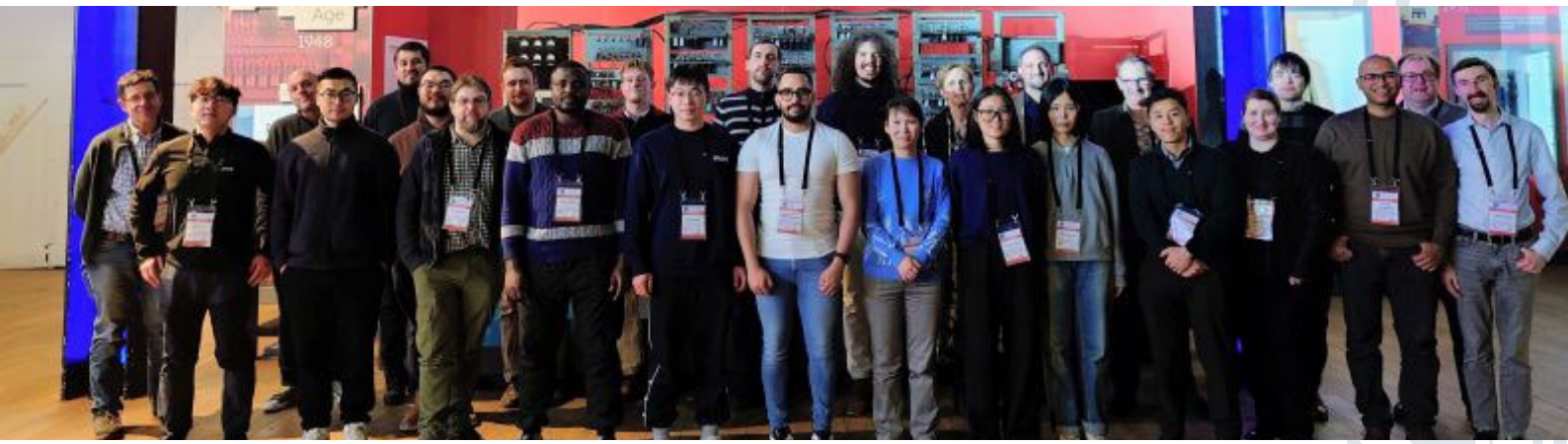
This workshop and hackathon focussed on efficient integration of SIRF/STIR/CIL with PyTorch. It was held from 7-9 April 2025 at UCL to enable use of AI/ML tools within the codebases, such as deep learning denoisers.

CCP-NC Workshop, May 2025

CCP-NC organised a 50-person, two-day workshop in Manchester bringing together some of the grand challenges in NMR crystallography with potential solutions in the form of machine learning (ML) capabilities. The meeting focussed on discussions between these two communities, with questions around the general model of interaction (e.g. collaboration vs training) as well as how to tackle particular scientific challenges together. The feedback collected after the workshop was positive, with many respondents appreciating the productive engagement between the two communities. The discussions also helped to shape the CCP-NC ML projects.

CCC-ParaSolS Network Events, May 2025 and January 2026

CCP-ParaSols held several network events throughout the past fiscal year – 14-16 May 2025 at the University of Edinburgh, 13-15 October at Abingdon, and 12 January at the University of Manchester, learning about the use of AI/ML with particulate solids simulations. They had a great turnout for all events with excellent talks and hand-on tutorials.



CoSeC Community Forum, June 2025

Our first forum of the year was held at the University of Sheffield, which saw a change in format, moving more towards the idea of the forum being an opportunity for discussion and collaborative knowledge exchange, rather than a way to provide a detailed overview of the technical research being conducted within each community.

The forum has evolved from the CCP Steering Panel meeting into a more wide-reaching meeting, that considers not only the amazing research happening within the CCPs and HECs, but also the strategic aspects of what research communities can do to help enable a stable and effective DRI.

We saw effective dissemination of the upcoming DRI landscape from the perspective of UKRI into the communities and a strong set of discussions about the best way to strategically position the communities to maximise their value for UK research. A highlight was during the round-table discussion session where a mixture of new and established community chairs, as well as UKRI representatives were able to discuss some fundamental ideas about what a community is and what good looks like in terms of research software development. Outcomes from these discussions can be found in the report of the meeting and offers a useful insight into current thinking and plans for improvement.

Read more about the report of the meeting

cosec.ac.uk/calendar/cosec-community-forum/june-2025/

SIG/CCP-NTH Annual Technical Meeting, June 2025

The SIG/CCP-NTH Annual Technical Meeting 2025, co-hosted by CoSeC, CCP-NTH, and Rolls-Royce was held at the Nuclear Skills Academy in Derby from 19–20 June.

Over 60 experts attended from across academia, industry, and government, with the meeting featuring a vibrant mix of contributions from the Universities of Manchester and Sheffield, Imperial College London, and STFC; industry partners such as Rolls-Royce and EDF, and public bodies including UKRI, NIRO, UKAEA, and UKNNL.

Together, they explored a series of engaging technical sessions on:

- Flow and Heat Transfer in Nuclear Thermal Hydraulics (NTH)
- Code and Methodology Development in NTH
- Novel Coolants & Fusion Reactor Thermal Hydraulics
- AI/ML Applications in NTH.

A forward-looking panel discussion took place on “The Potential Utility of AI in Nuclear Thermal Hydraulics and the Associated Challenges”. The discussion brought together diverse perspectives on AI integration in NTH from academia, industry, and regulators, highlighting both the opportunities and practical challenges in this evolving area.

CCP-UKNR workshops, June and December 2025

UKNR ran two very successful workshops, which were held from 17-19 June 2025 at the historical Gregynog Hall venue (which is the site of the first ever numerical relativity workshop held in 1980). These workshops brought together the members of the CCP-UKNR community, CoSeC and international stake holders. In particular, the latter included Katherine Riley, who is the Director of Science for the US Argonne National Lab (which operates the first exascale machines Aurora and Frontier), and Mark Wilkinson who is the Director of DiRAC. The goal of the workshop were threefold:

- Science: Discuss the state of the art of numerical relativity, and the code development and strategies to confront the increasingly challenging precision requirements dictated by upcoming experiments in particular the international LISA space-based mission in which the UK is a major partner
- Strategic Planning: Understand the present and future digital landscape for the next 5-10 years, and the challenges it will bring to numerical relativity
- Community Building: Discuss and formulate actions that will strengthen the foundations of a good community.

Read more about the workshop, Numerical Relativity 2025: Towards the Next Generation

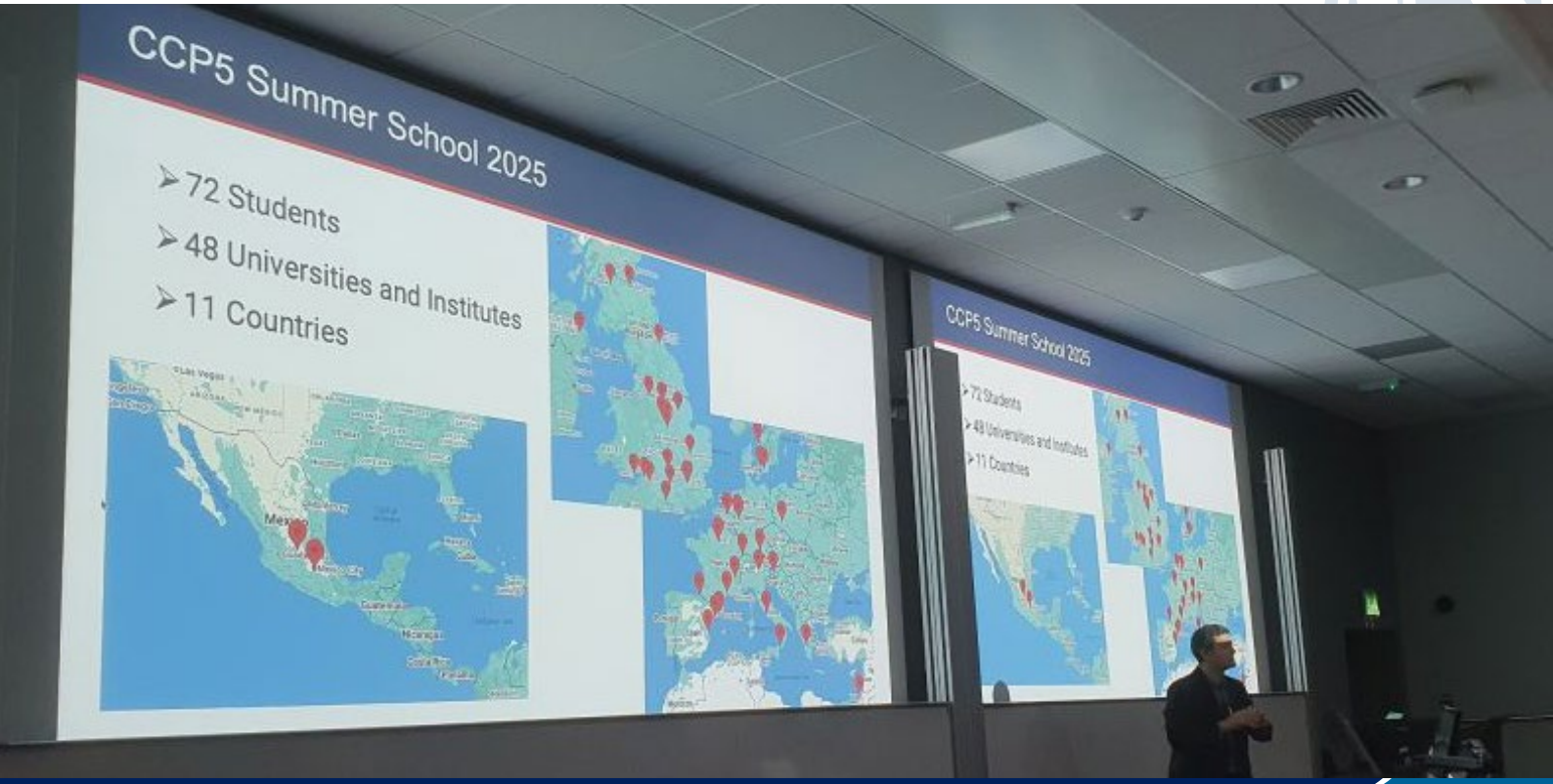
sites.google.com/view/nrgregynog/

CCP5 Summer School, July 2025

The CCP5 Summer School 2025 was an intensive training program focused on molecular and materials simulation, specifically designed for newcomers to the field, such as PhD students. The school, organised by CCP5 and sponsored by CECAM with support in teaching from CCP9, MCC, UKCOMES and CCPBiosim for advanced courses, took place from 20-31 July 2025, at Newcastle University.

The program was structured in three main parts to provide a comprehensive and progressive learning experience. It began with a two-day programming course, where participants could opt for either Python or modern Fortran to build a necessary computational foundation. This was followed by the core of the school, consisting of five days dedicated to the basics of molecular simulation. These foundational lectures and extensive practical sessions covered critical topics like Statistical Mechanics, Molecular Dynamics, Monte Carlo Methods, and different Free Energy Methods, aiming to solidify the theoretical background and practical skills in computational chemistry and physics. The final three days were devoted to advanced courses, allowing students to specialise in key emerging and established areas of simulation. These options included Mesoscale Methods, Ab Initio (First-Principles) Simulations, Biomolecular Simulation, and the application of Machine Learning for Interatomic Potentials.

Overall, the school's purpose is to provide early-career researchers with the essential skills and insights required to successfully conduct research in molecular, liquid, and solid-state simulations. This year we had 72 students from all Europe, US, Mexico and UK. Best oral presentation winner was Akanksha Nawani, Sorbonne University, France and posters winners, Nga Man Cheng, University of Nottingham, UK, Gustave Szczepan, CEA, France, Sarah Haggenmueller, Technical University of Munich, Germany, Matthew Ludwig, University of Bristol, UK.



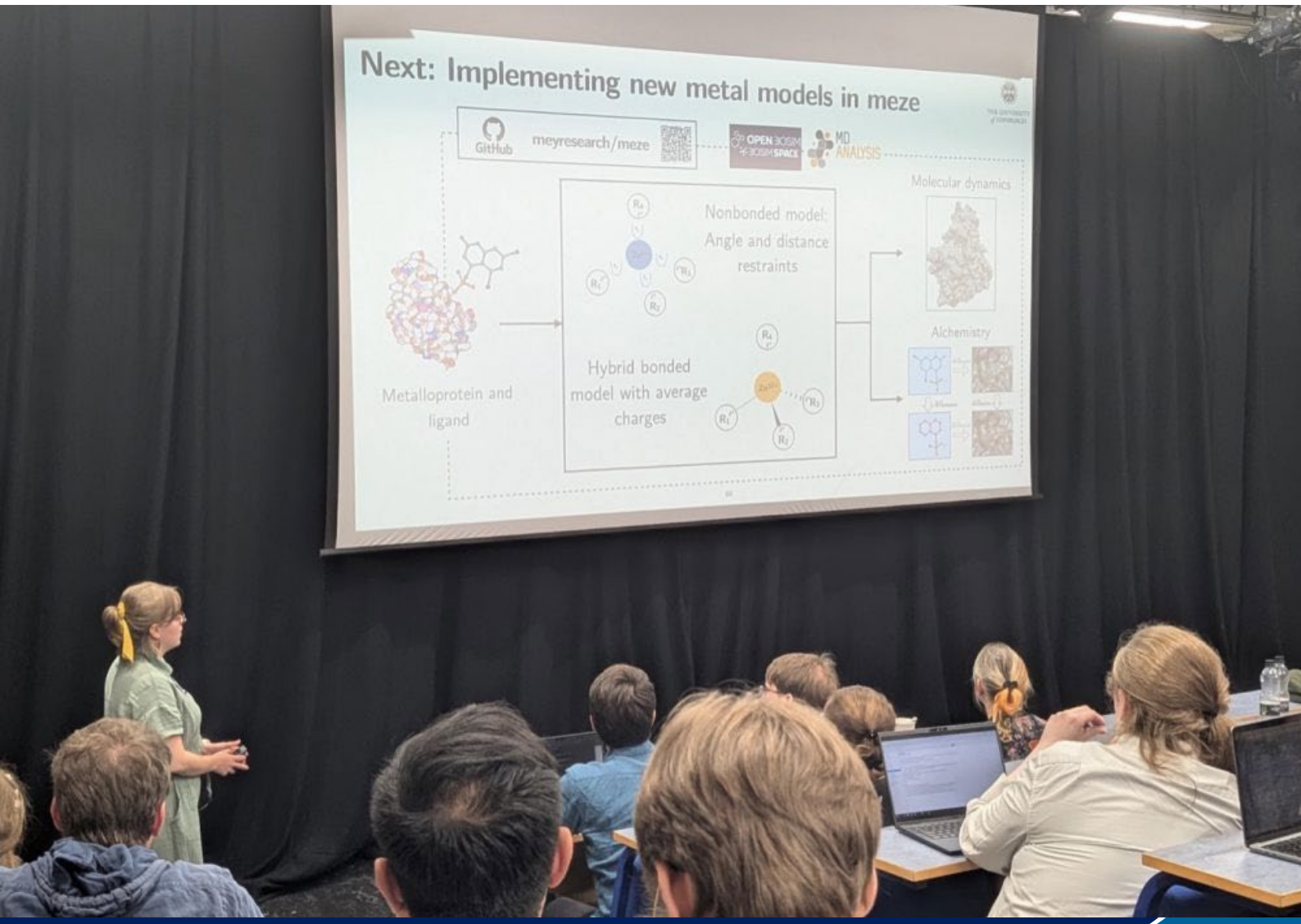
CCPBioSim talks and DRIIMB webinars, July 2025-March 2026

A DRIIMB seminar on PDB-IHM (9 July 2025) introduced community data resources supporting integrative and hybrid structural models used in biomolecular research.

An industry talk by Ted Smith (5 November 2025) discussed career development within the life sciences sector, followed by a DRIIMB seminar on BioSimDR (7 November 2025) which introduced infrastructure designed to support FAIR data sharing for biomolecular simulations. In early 2026, further industry and research webinars were held, including an industry talk from Sygnature Discovery (15 January 2026) and a DRIIMB webinar by Helen Berman (22 January 2026) on structural biology data resources. Additional webinars included an industry talk from Schrödinger (12 February 2026), and DRIIMB webinars on mass-spectrometry-based structural modelling (19 February 2026), and artificial intelligence in bioscience through the AIBIO-UK network (5 March 2026). The average attendance across the industrial seminars was approximately 120 people.

11th Annual CCPBioSim Conference, July 2025

The 11th Annual CCPBioSim Conference: Frontiers in Biomolecular Simulations (14–16 July 2025 attended by 104) showcased recent methodological advances and applications of biomolecular simulation.



Energy Efficient Computing Workshop, September 2025

On 15-16 September 2025, an Energy Efficient Computing workshop was held at Harwell Campus, organized by STFC Theme Lead for Mathematics Dr Tyrone Rees, Software Engineers Jessica Huntley and Adam Greenbank, and CCP-DCM Project Lead Dr Hussam Al Daas.

The workshop was primarily aimed at software development teams embedded within our communities at CoSeC. The sessions revolved around four key themes: Qualitative Algorithms, Community, Hardware, and Quantitative Practice and was designed to share knowledge and start conversations around making energy-efficient choices.

Dr Tyrone Rees (left), STFC Theme Lead for Mathematics opened the workshop and our Director, Dr Stephen Longshaw talked about CoSeC, current developments and plans for the future and a summary of each talk is available below.

"It was great to see high levels of engagement across different communities and user groups during the workshop, which sparked interesting conversations and highlighted the importance of taking a multi-disciplinary approach to embedding energy-efficient computing practices. The high-quality talks also stimulated some great discussions as part of our breakout sessions, giving us lots of ideas to take forward in the next phase of our project."

Jessica Huntley

Co-organiser

Read more about the workshop and the talks involved

tinyurl.com/4xz6p842

CECAM/ALC/CCP9 Spectroscopy Masterclass, September 2025

CCP9 lead the organisation of an important networking and training event in theoretical spectroscopy: the “CECAM/ALC/CCP9 Spectroscopy Masterclass” was held at STFC Rutherford Appleton Laboratory, Didcot, 2-5 September 2025 and brought together experimentalists from the large scale facilities and theoreticians working in modelling spectroscopy to learn state-of-the-art calculation methods and discuss future challenges and opportunities. The school, which was funded by CECAM and the Ada Lovelace Centre, as well as CCP9, attracted about 60 participants from across Europe and beyond.

CCP-TEPP Knowledge Exchange Meeting, September 2025

Following a series of scoping and discussion workshops throughout the first half of 2025, this meeting brought together the various parts of the community to present work on topics of common interest. 36 participants (including 13 invited speakers) presented and discussed topics where there are common challenges across the field, as identified from roadmapping workshops earlier in the year. Topics discussed included computational infrastructure, automation and reproducibility of data analysis, accelerators and performance portability, software maintainability and code quality, and applications of quantum computing, and machine learning technologies.

CCP-WSI Blind Test Series 5 workshop, September 2025

The CCP-WSI Blind Test Series 5 workshop with topic sloshing in cylindrical tank was held on 19 September 2025. 41 participants from all around the world attended this workshop, where different numerical methods were presented and discussed. The physical data used in the blind test was shared and the dataset included the time series for the assessment criteria, along with video data for each of the cases.

CCPBioSim Training Week, October 2025 and workshops

CCPBioSim ran their annual training week of hands-on workshops in basic bimolecular simulation techniques from 13-17 October, at Halifax Hall, Sheffield.

This in-person event provided a practical introduction to fundamental methods in modern bimolecular simulation, including setting up and analysing MD simulations of proteins (both soluble and membrane-bound), ligands, and nucleic acids.

Additional workshops and seminars included an industry talk from Oxford Drug Design (23 July 2025), the CECAM Flagship Workshop Entropy of Soft Matter (27–29 August 2025 and attended by 30). This meeting in Vienna, Austria was co-sponsored and organised by CCPBioSim and arranged to coincide with the release of their new flagship software (CodeEntropy), which was unveiled at the conference. 30 people came to present and discuss entropy and the software used to calculate entropy from simulations. A further industry talk from AstraZeneca (24 September 2025), and a presentation from FACCTs (8 October 2025) exploring high-accuracy quantum chemistry methods.

CCP-AHC Workshop, October 2025

A pilot training workshop on AI tools for working with scanned documents was delivered at University of Luxembourg, Centre for Contemporary and Digital History (C2DH) on 14 October 2025. The workshop showed how FAIR image publication standards (IIIF) and open-source tools (Voxel51's fiftyone) can be used together to run computationally intensive AI workflows using cultural heritage datasets without code.

Read more about C2DH

tinyurl.com/4r9ajcft

CoSeC Community Forum, November 2025

Held on 5 November 2025 at Durham University, the forum was hosted by the Chair of CCP-AHC, Dr Eamonn Bell. The agenda was designed to explore wide-reaching DRI topics that are particularly relevant for communities, such as identifying impact and related metrics beyond traditional research outputs, as well as inclusivity as a driver for better research communities.

Alongside these important topics, the future of the UKRI research community model was a key topic, with this meeting timed at the point just ahead of the next phases for both the CCPs and HECs. The meeting allowed community chairs to receive the latest information directly from all UKRI Research Council representatives, DRI, SSI and CoSeC, while directly feeding back. Discussions were also held the developing Forum format and community aspirations and priorities for elective future funding given the new compute resource support landscape.

"I left this meeting in Durham more enthused than ever about the state of the computational community landscape within the UK. Communities continue to adapt, grow and thrive. The total number of funded CCPs and HECs that CoSeC works with directly now sits at 25, with further communities out there. Following our recent call to create scoping projects for new CCPs, the landscape is becoming truly cross-UKRI in nature and the tangible outputs seen from this model can only be described as world-class. I have no doubt that what we have now is fundamentally the right approach and it is clear from recent opportunities that it is adaptable to whatever UKRI needs."

Dr Stephen Longshaw

CoSeC Director

Read more about CCP-AHC

ccpahc.ac.uk/

CoSeC Annual Conference, December 2025

The 2025 CoSeC Annual Conference took place on 3 December at Manchester Central Convention Complex, as part of the wider Computing Insight UK Conference. The official conference proceedings are now available.

The conference, now in its fifth year, promoted the research and achievements of the CoSeC communities for the past year. Collaborators presented on a range of subjects and we were delighted to introduce our second cohort of CoSeC Fellows.

This conference reflects the achievements of the past year and the body of research that addresses the increasingly complex scientific computing challenges that we face today. Over the last five years of the CoSeC Conference being included within CIUK, we have seen a continual increasing in quantity and quality of submissions, as well as the diversity in topics. The conference provides a key moment in the UK calendar for computational research communities to come together and discuss collaboration and areas where they cross-cut. This year's event was the biggest, most successful to date and a great indicator for the future of collaborative community-driven research within the UK.

This year the key themes included; Modelling, Simulation & Reconstruction; Scientific Reproducibility; Data Stewardship and to exploit the new hardware Accelerated Computing.

Cross cutting principles presented included how to exploit current HPC facilities available to the CoSeC communities, as well as emerging and next-generation national facilities considering governance and data management; and then key technical issues surrounding the future of a sustainable research computing.

"The ability to just wait for computation power to increase is tempting", says Conference Chair, Dr Martin Turner, University of Manchester. "But the CoSeC communities have shown the advantages to strive now to consider how to best use current and exploit future computational abilities. Software development both technically and governance need to continue to evolve at a similar rate to hardware progress."

Read more about Computing Insight UK Conference

ukri.org/CIUK

Watch Computing Insight UK Conference videos

tinyurl.com/55knnvd5

UK AI for Turbulence Workshop, January 2026

The UK AI for Turbulence Workshop was held at the British Library in London from 26-27 of January 2026, with over 180 participants. The aim of this workshop was to bring together multidisciplinary stakeholders from industry and academia to establish state-of-the-art AI applications in turbulence, showcase UK expertise and capabilities, and identify key research priorities and collaborative opportunities. The workshop featured a mix of presentation formats, including keynote lectures from leading researchers, interactive panel discussions, and e-posters for young academics in order to encourage deep engagement between participants from different backgrounds. The event was designed to maximise networking opportunities and facilitate new collaborations. This workshop will directly inform the development of a position paper around AI for Turbulence to be published in the Data-Centric Engineering. A survey will follow to gather the view of the community around how AI can be used for turbulence research. This event was sponsored by Cambridge University Press, Data-Centric Engineering, the UK Turbulence Consortium and the CCP Turbulence (thanks to funding from UKRI and the Digital Research Infrastructure (DRI) Programme.

CCP4 Study Weekend, January 2026

The 2026 CCP4 study weekend was entitled “Ligands in Focus: Decoding Ligand Binding in Modern Structural Biology” and held as a hybrid event from 7-9 January 2026, enabling people to choose whether to attend in-person or virtually. The in-person event was held at the East Midlands Conference Centre, Nottingham, UK.

The weekend was a mix of cutting-edge science, in-depth presentations, a discussion panel, poster-sessions, hands-on tutorials, and plenty of opportunities for social interactions.

CCPSyneRBI’s Symposium on AI and Reconstruction for Biomedical Imaging

CCPSyneRBI’s Symposium on AI and Reconstruction for Biomedical Imaging was held from 9-10 March 2026 in London.

This two-day symposium featured internationally-leading researchers covering recent advances in AI and image reconstruction for biomedical imaging, intended to enhance UK and international networking, research progress and education in this important area. The symposium was part of the EPSRC funded computational collaborative project in synergistic reconstruction in biomedical imaging (SyneRBI).

The symposium included a dedicated session on the PET Rapid Image Reconstruction Challenge 2 (PETRIC2).

Read more about PETRIC2

ccpsynerbi.ac.uk/events/petric2/

Fellows

In 2024, CoSeC welcomed its first cohort of eight CoSeC Fellows, followed in 2025 by a second cohort of ten. Each Fellow is an ambassador for the Centre, highlighting the benefits of CoSeC and the CCP model, and making scientists and researchers aware of the world leading activities undertaken through CoSeC's work.

CoSeC Fellows help to highlight the work of CoSeC in supporting the advancement of computational research by developing and strengthening software to analyse and solve increasingly complex problems in multiple disciplines across UKRI – arts, humanities, physical sciences, engineering and more. In return, CoSeC Fellows gain access to, and learn from, interactions across a wide range of research areas. Fellows gain experience of working in a world-leading scientific environment, increasing their skills and knowledge. They have the opportunity to raise their own personal profile and have the prospect of creating future educational and employment openings as they develop their careers.

The 2025 cohort includes:

Irufan Ahmed, Senior Software Engineer, Imperial College London, whose work focuses on the development and maintenance of computational research software. He also provides support for researchers on software engineering best practices for sustainable and reproducible research.

Kemal Atalar, Research Associate, King's College London, whose research lies at the intersection of physics, chemistry, and computation, where he develops new methodologies for first principles modelling of molecular and material systems. He focuses on reduced-order and surrogate models that accelerate the evaluation of electronic states across nuclear configurations.

Chandan Bose, Assistant Professor of Aerospace Engineering, University of Birmingham, is a subject expert in computational fluid-structure interaction (FSI) and leads the university's Bioinspired Fluid-Structure Interaction Laboratory. His group conducts cutting-edge research on the computational modelling of biomimetic engineering system.

Shreyank Narayana Gowda, Assistant Professor, University of Nottingham, is a researcher specializing in deployable computer vision research with a focus on data-efficient and memory-efficient learning methodologies, across diverse datasets such as images, videos, and medical data strongly motivated by how we as humans see and learn with a long-term goal of making AI sustainable.

Andrea Nóvoa, Assistant Professor, Imperial College London, focuses on developing real-time digital twins for engineering systems to enhance real-time monitoring, prediction, and control in engineering. Specifically, she develops robust computational methods that improve the understanding and management of complex dynamical phenomena such as thermoacoustic instabilities in low emission aeroengines, or aeroelastic instabilities in wind turbine blades.

Martin Rey, Lecturer, University of Bath, is a computational astrophysicist driven by a fascination with how galaxies come to be. His research uses large-scale cosmological simulations to trace the complex interplay of gas, stars, and dark matter across billions of years of cosmic time. He aims to uncover the physical processes that shape galaxies and provide theoretical insight for observations from instruments such as the James Webb Space Telescope.

Alejandro Jimenez Rios, Lecturer, University of Bath, leads the History, Conservation, and Management Cluster in the University's Department of Architecture & Civil Engineering. His work sits between structural mechanics, cultural heritage, and digital technology where he often finds himself trying to make these worlds speak to each other.

Jemima Tabeart, Assistant Professor, TU Eindhoven, is in the University's Computational Science group and her research interests lie at the intersection of numerical linear algebra and data assimilation for high-dimensional applications. She has collaborated with the Met Office and CERFACS to develop new mathematical approaches for practical applications in numerical weather prediction and oceanography.

Miquel Miravet-Tenés, Research Fellow, University of Southampton, focuses on studying binary neutron star mergers through numerical-relativity simulations. He aims to understand the role of small-scale turbulence and finite resistivity in the dynamics of these systems and their multimessenger observables.

Esther Turner, Senior Research Software Engineer, National Oceanography Centre, has a background in particle physics, having obtained her DPhil in this field, and she has since worked in research software engineering across fields including climatology, meteorology, national infrastructure and, currently, oceanography. She provides software development expertise to a wide range of projects and is also involved in building a Data Science Platform, which will be an underpinning piece of infrastructure at NOC.

The 2024 Fellows concluded their fellowship in December 2025:

Michael Bane, Professor of Green Engineering, Manchester Metropolitan University, focused on green software engineering, including how to reduce the carbon emissions of computing in support of net zero ambitions. Michael worked to help accelerate uptake of Green Software Engineering principles across the CCPs and the wider software engineering communities, in support of UKRI DRI Net Zero commitments.

Ignatius Ezeani, Research Fellow, Lancaster University, focussed on the efficient adaption of existing natural language processing tools and techniques to deal with the challenges of integrating the majority of the low-resource languages in a globalised world for task-oriented systems. Dr Ezeani's work directly aligned with the core objectives of CoSeC in building strong research communities of computer scientists for effective collaborations.

Qian Fu, Research Fellow, University of Birmingham, a vision to create an open-source Python tool that integrates large-scale data efficiently, empowering researchers to run complex models that support urban planning and disaster mitigation. The Fellowship allowed Qian to enhance his current work on large-scale transport network modelling, analysing the impact of extreme weather on transport resilience and people's travel behaviours.

Christian Gutschow, Senior Research Software Developer and Particle Physicist, UCL, focussed on sustainable software development and creating software that delivers simulations to model data from CERN's Large Hadron Collider. With a strong history of working closely with Monte Carlo (MC) generator authors, Christian is leading the UK's efforts in the development of sustainable and scalable MC production workflows to meet the challenges ahead.

Tuomas Koskela, Principal Research Software Engineer, UCL, focussed on scientific software that takes advantage of High-Performance Computing facilities. During his Fellowship, Tuomas worked towards creating long-term capability of understanding code and system performance across communities in UKRI, organising and attending knowledge exchange events to discuss best practices in benchmarking HPC applications and systems.

James Parkhurst, Postdoctoral Research Associate, Rosalind Franklin Institute, is currently developing an independent research programme using simulation and modelling approaches for the specification of Transmission Electron Microscope (TEM) hardware and system requirements, offline optimisation of data acquisition parameters and determination of data collection strategies for cryo-ET. He had already collaborated closely with researchers and software developers within CoSeC, including CCP4 and CCP-EM and throughout his Fellowship, worked on implementing software for the alignment and reconstruction of cryo-ET data not currently catered for by existing software.

Christopher Woodgate, EPSRC Doctoral Prize Fellow, University of Bristol, focuses on understanding aspects of the physics of multicomponent alloys and high entropy materials. He is actively involved in the CCP9 and CCP5 communities due to the multiscale nature of his research. Throughout his Fellowship, Christopher highlighted the benefits of networking and collaborative development of community codes for the acceleration of research projects to the wider academic community.

Chengcheng Xiao, Postdoctoral Research Associate, Imperial College London, is focused on implementing Brillouin zone (BZ) sampling in ONETEP – a UK based density functional theory software that is able to simulate very large systems (tens of thousands of atoms) at a quantum mechanical level. The Fellowship enabled Chengcheng to attend conferences and workshops to disseminate his developments to the scientific community, helping him build and expand a stronger user/developer community around ONETEP.

Read more about ONETEP

onetep.org/


PSI-K 2025
August 25-28
Lausanne
Switzerland

Awards

CoSeC Impact Award for 2025

The 2025 CoSeC Impact Award was awarded to Dr. David Lusher of the Japan Aerospace Exploration Agency (JAXA) for his exceptional contributions to the scientific community.

The CoSeC Impact Award recognizes individuals whose work has had a significant positive impact on the scientific community, in close collaboration with CoSeC and the communities we support.

Dr Lusher is the co-creator and lead developer of OpenSBLI, a widely used open-source software package that has become essential for researchers in the field of Computational Fluid Dynamics (CFD). The code is used by researchers and organizations worldwide, and key UK research communities, such as CCP Turbulence and UKTC, who rely on it heavily.

David's work has had an immense impact, providing an open alternative to closed-source codes and fostering a more collaborative research environment. As one of our panellists noted, code development is a contribution that academia has traditionally overlooked, and we are proud to recognize its profound importance with this award.

"I am honoured to receive this prestigious award from CoSeC. The main development of OpenSBLI was undertaken during my PhD at the University of Southampton with support from members of the CCP Turbulence and UKTC communities. Since joining JAXA, I have extended the capabilities and scope of OpenSBLI through collaborative research with the University of Southampton, NASA Langley, and other international partners. This work has enabled large-scale high-fidelity simulations of complex fluid flow phenomena, such as transonic airfoil buffet, that were previously out of reach. CoSeC-supported OpenSBLI training workshops have given me the opportunity to engage with new users of the code in support of their research projects and maintain strong links with CFD research within the UK. I am grateful for the support from staff at STFC and look forward to seeing future research applications on the next generation of UK high performance computers using open-source CFD codes such as OpenSBLI."

Dr David Lusher

Co-creator and lead developer of OpenSBL

"We are delighted to offer this award to David. OpenSBLI, the code that David has developed is a key one that has already been extensively used in a number of our communities, including CCP Turbulence and UKTC. It is a key UK code that was used as part of the development suite for our current national supercomputer ARCHER2."

Dr Stephen Longshaw

Director of CoSeC

Read more about David's career

cosec.ac.uk/impact/winner-of-2025-cosec-impact-award-winner-announced

CoSeC Staff Impact Award for 2025

Dr Alin Elena, a computational scientist leading the Data-Driven Molecular and Materials Science Group in the Scientific Computing Department, was awarded the 2025 CoSeC Staff Impact Award. Alin is a member of the CCP5 and CCP-QC communities and received the award for enabling, through technical expertise, the delivery of extended hands-on sessions for several CoSeC training events in 2025, including the long-running and very well respected annual CCP5 Summer School.

CoSeC Early Career Award for 2025

Dr Joel Greer was the inaugural recipient of the CoSeC Early Career Researcher Award for his work investigating methods to observe molecular motions from cryo-electron microscopy. Joel is a member of the CCP-EM community and is also part of the newly formed DRIIMB consortium. Joel's current work will ensure that STFC Scientific Computing and CCP-EM remain at the bleeding edge of cryoEM software development.

Funding Opportunities

CoSeC supports a wide range of computational scientific and engineering communities, through software development, user support and training, and management of scientific data.

The funding enables the advancement of computational research by developing and strengthening software to analyse and solve increasingly complex problems in multiple disciplines – arts, humanities, physical sciences, engineering and more.

CoSeC itself is funded as a cross-UKRI activity with delivery through STFC National Laboratories. The Centre receives support from the EPSRC, BBSRC, MRC research councils and from central UKRI via its Digital Research Infrastructure programme.

Over recent years, CoSeC has awarded over £5m of funding to its communities through a number of funding calls, a fellowship programme and an ongoing collaboration visit funding opportunity.

In November 2024, CoSeC awarded £2.7m of funding to our current CCP communities in the form of a bridging funding award. This funding was designed to bridge these communities from their existing council-specific position to one aligned with that of the wider UKRI DRI to enable a strong cohort of cross-UKRI organised community activity to support the UKRI ambition around its research infrastructure. This would then for successful applications one FTE of CoSeC support effort was also included.

In January 2025, these bridged communities were invited to apply for additional funding up to a total value of £400,000. This funding was made available to ensure workplans remained achievable by enabling available RTP effort across the communities where it was unable to be resourced within CoSeC at the time required.

Alongside these calls, funding to the value of £1.125m was enabled through a **"Collaborative Computational Communities: towards new CCPs"** call to develop and proliferate the Collaborative Computational Project (CCP) model across research communities within UK Research and Innovation (UKRI). This created a strong and stable landscape of communities to support the concept of research computing software as an infrastructure.

This funding came via STFC from UKRI's Digital Research Infrastructure (DRI) programme and was curated by CoSeC. The expectation is that CoSeC will be a part of the plans and activities within each community, providing a collaborative relationship between them. The purpose of this funding is to enable community scoping to identify and define viable new CCPs that can be incorporated into the existing rich community landscape, expanding its overall research remit and the reach of the collaborations it can provide.

The CoSeC Fellowship Programme has now successfully awarded eighteen fellowships over two cohorts in 2024 and 2025. Each fellowship includes up to £3000 in fellowship funding to be used to support the activities of the selected Fellows. Each, in turn become ambassadors for CoSeC whilst benefitting from excellent networking opportunities and professional support and advice from CoSeC staff.

CoSeC also offers financial support for community collaboration visits. The funding is available on a rolling basis – applications are accepted throughout the year as required or until overall budget is allocated.

This is available to encourage and promote collaborative visits with colleagues and project partners from CoSeC funded communities. These visits enable knowledge exchange and accelerate community-driven development of research software related to CoSeC and the collaborative computational communities.

The funding can be used to cover costs such as travel, accommodation and living costs encountered during the visit. This is not be delivered as a grant, but instead the CoSeC Programme Office helps by making travel arrangements or by reimbursing expenses up to the award limit.

The goals of this funding are to:

- Enable visits to collaborate directly with CoSeC staff at UKRI STFC's National Laboratory locations
- Enable intercommunity knowledge exchange within the UK
- Provide support for UK researchers within the collaborative computational communities to engage in international knowledge exchange.

Read more about CoSeC funding opportunities

cosec.ac.uk/funding

Case Studies

Delivering state-of-the-art training worldwide:

How CoSeC developed high demand software during an international crisis

A challenge facing STFC Scientific Computing is delivering state-of-the-art software to institutions with outdated systems unable to accept the latest developments. Its Computational Science Centre for Research Communities (CoSeC) Programme can provide this essential continuity to upskill new staff and deliver cutting edge computing tools through CCPs (collaborative computational projects). One of these, CCPBioSim, has developed a unique platform that has successfully been taken up on a large-scale globally.

The Challenge

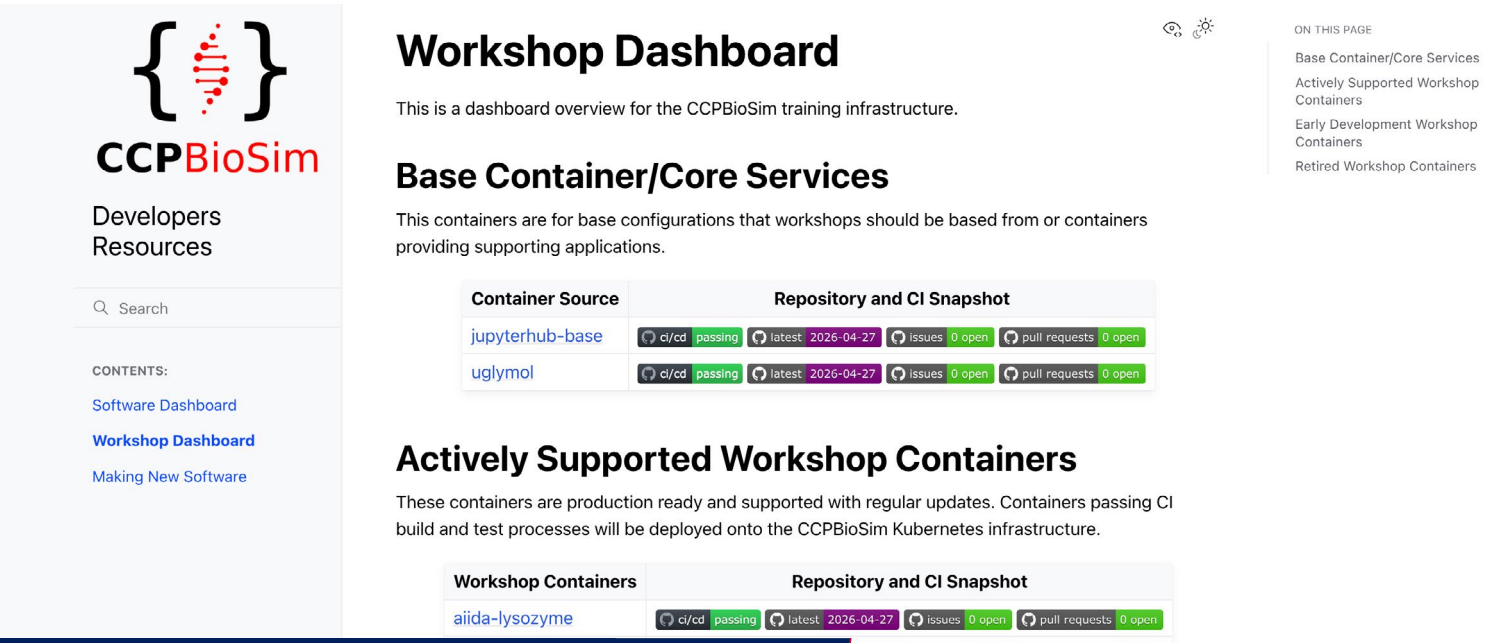
An issue that the communities within CoSeC continue to face is that, despite working on cutting-edge software tools, it is often found to be the case that an institution or organisation's systems are too old to adequately run the latest software. Often installation is blocked, with the system either presuming a security threat or indicating licencing issues. This has led to frequent delays in any attempt to get training established and, in some cases, the very software brought in to help improve training could not be run due to insurmountable IT policies.

The Approach

In 2015, Jupyter Notebook launched, which was aimed primarily at teaching software development. The ability to run various software languages directly in a web browser was a game-changer and with the training also using various languages, such as Python, it was a natural fit for CCPBioSim Training Resources, which uses simulations to further the understanding of the biological functions of proteins. The benefits were instant. Advanced software developers could create their own training environment offline, months ahead of the training workshop, leaving ample time to test and develop different devices. From a user perspective, all the trainee needed was a web browser. When the world went into lockdown during the COVID pandemic, the team at Jupyter began looking for training materials to do their first simulations. With CCPBioSim hosting training courses on Jupyter Notebook, suddenly their attendee numbers jumped from 70 to 700!

CCP BioSim Training Week, 21st September 2022

> **“Scientists were stuck at home during lockdown and unable to go into the lab, so they could run our software on their laptops with no technical requirements beyond a web browser. It meant we could deliver fantastic training during an international crisis and teach state-of-the-art viral simulation techniques.”**
>
> **James Gebbie-Rayet**
>
> CoSeC Technical Lead for CCPBioSim, STFC Scientific Computing



Screenshot of CCP BioSim Workshop Dashboard

The Benefits

CCPBioSim software engineers now travel to conduct training in countries with developing economies where advanced software programs and supercomputers are unavailable, so far delivering training in South America, Asia and Africa.

Further advantages included the ability to log in and log off without losing progress, and the availability of the team to answer questions on an ongoing basis, as opposed to an in-person workshop with the trainer only there for the day.

With such high demand for training, the challenge now for the team was to not only respond to this demand but also to adhere to its promise to deliver state-of-the-art training. Software packages are being continually updated and the team is constantly updating to the latest version. Over twenty courses are now available with hundreds of different software dependencies. Analytics have revealed a total of 20,000 training sessions delivered remotely since 2020.

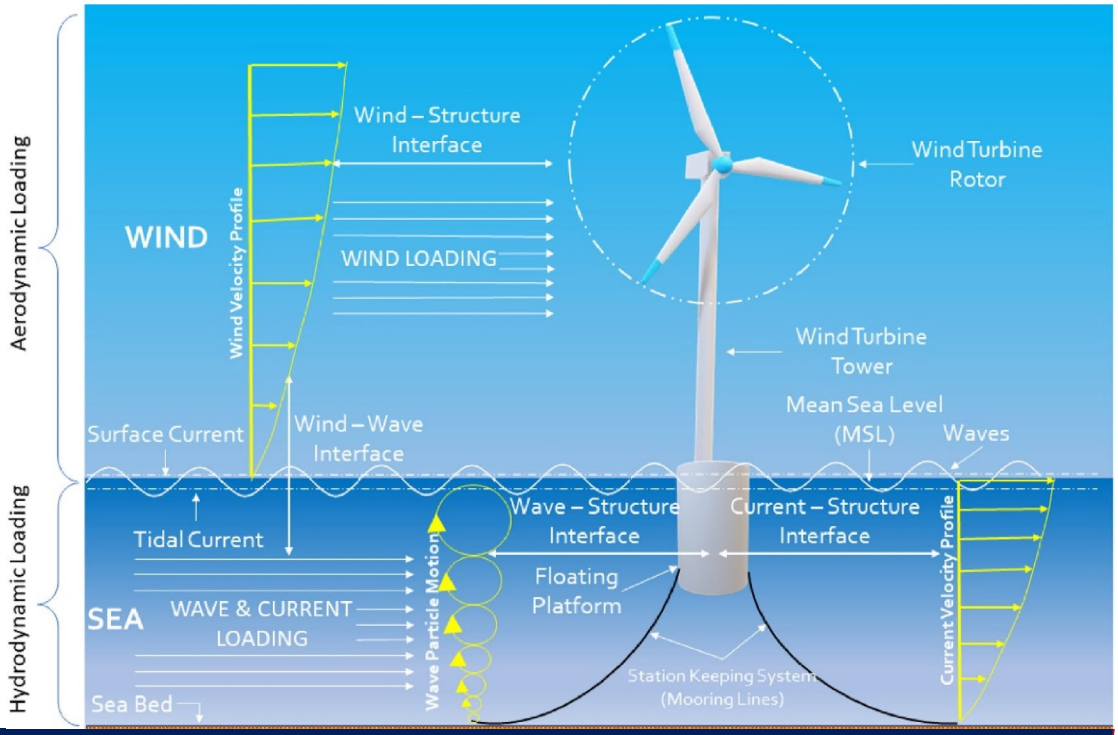
Next steps

The team plans to build a new iteration of the platform and implement a suite that will test each course for viability and simultaneously update to the latest software version. CCPBioSim will have a training resource that is self-testing and self-deploying, automatically updating and ready at one's fingertips – likely one of the most advanced systems in the world. Already at an advanced stage with five years' worth of feedback and development, the platform will be hugely beneficial to institutions and organisations to use for their own training programmes. It has been continually tested and developed by people expert in both scientific computing and software development.

> **"You would never be able to do anything like this without CoSeC. The fact is that we can organise academics across the country to create material for a common purpose – in this case, upskilling. Today scientists are trained more in laboratory conditions, rather than in computing, so they need to be trained in these skills. Every university has to train their own scientists, and we have the capability, expertise and technology to deliver the training and enable them to quickly move forward together."**
>
> **James Gebbie-Rayet**
>
> CoSeC Technical Lead for CCPBioSim, STFC Scientific Computing

Addressing the UK's clean energy goals: How multiscale computer modelling can benefit wind farms

From turbulent ocean waves acting on offshore structures to detailed heat transfer within cryogenic systems, modern engineering and scientific challenges require increasingly sophisticated modelling that spans multiple physical domains and time scales. STFC Scientific Computing's CoSeC (Computational Science Centre for Research Communities) aims to create such modelling by delivering cutting-edge computational tools through collaborative computational projects (CCPs). One of these, CCP-WSI (Wave Structure Interaction), has collaborated on a code-coupling tool that not only directly addresses this challenge but will also hugely benefit the wind turbine industry in pursuit of renewable energy for a cleaner world.



Review of floating wind turbine damping technology

Tian, H., Soltani, M. N., & Nielsen, M. E. (2023). Review of floating wind turbine damping technology. Ocean Engineering, 278, 114365.

The Challenge

The development of new computational models and the integration of new techniques, such as AI and machine learning, are required to meet the rising demand for adaptable modelling in traditional scientific and engineering simulations.

An effective way to achieve this is with simulation codes from different disciplines that work together by using solvers (programmes that use mathematical or logical problems to reach a solution). However, in practice, coupling solvers is often complex and time-consuming. A solver is typically developed independently, with its own code architecture, numerical methods, data formats, and communication protocols. Therefore, enabling two codes to exchange data efficiently can require major code modification, undermine reproducibility and hinder progress across research communities.

Read more about Wave Structure Interaction

ccp-wsi.ac.uk

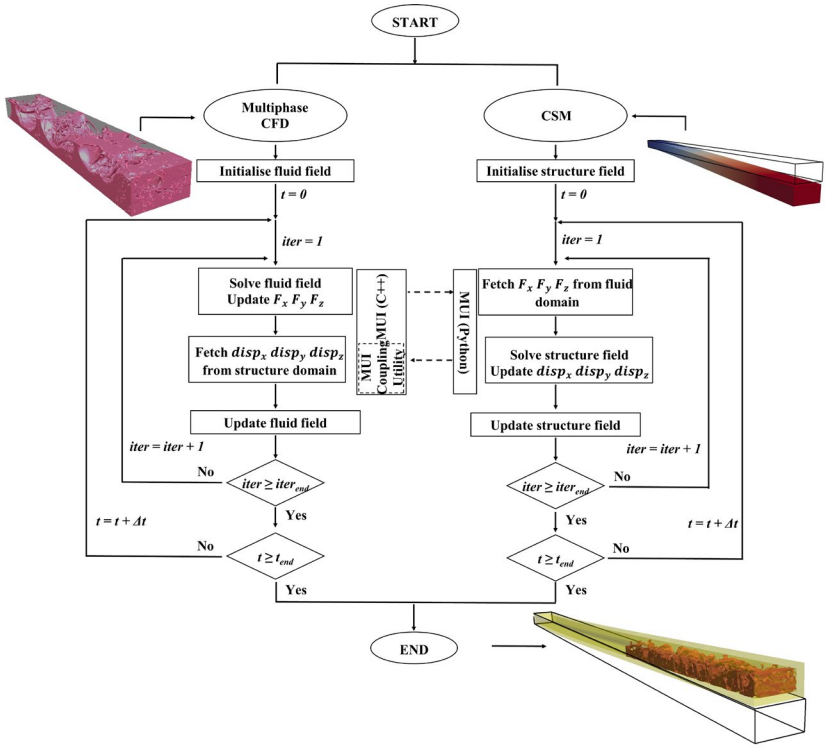
The Approach

Multiscale Universal Interface (MUI) is one of the code coupling tools that can address this challenge. A joint effort between Brown University, Lawrence Berkeley National Laboratory, Science and Technology Facilities Council (STFC) and IBM Research, MUI is a computer programme designed to facilitate concurrent coupling between diverse solvers with minimal disruption to their existing structure.

MUI provides a unified and efficient communication framework based on a message passing interface (MPI), which allows independently developed codes to exchange data during runtime. Its design ensures ease of integration and portability across computing environments.

Open Field Operation and Manipulation, known as OpenFOAM, is one of the world's most widely used open-source computational fluid dynamics (CFD) software, with a global community of more than 25,000 users across academia and industry. It is the de facto standard in many CFD-based studies, ranging from aerodynamics and heat transfer to multiphase and ocean engineering applications.

Through CoSeC, the STFC MUI team worked closely with OpenFOAM developers at OpenCFD Ltd to lower the technical barriers for coupling this software with third-party simulation codes.



Schematic of the MUI-powered open-source framework

Image credit: W. Liu, O. A. Mahfoze, S. M. Longshaw, A. Skillen, D. R. Emerson, Simulating slosh induced damping, with application to aircraft wing-like structures, Applied Sciences 12 (17) (2022) 8481.W. Liu, O. A. Mahfoze, S. M. Longshaw, A. Skillen, D. R. Emerson, Simulating slosh induced damping, with application to aircraft wing-like structures, Applied Sciences 12 (17) (2022) 8481.

Read more about Multiscale Universal Interface

mxui.github.io

Read more about Open Field Operation and Manipulation

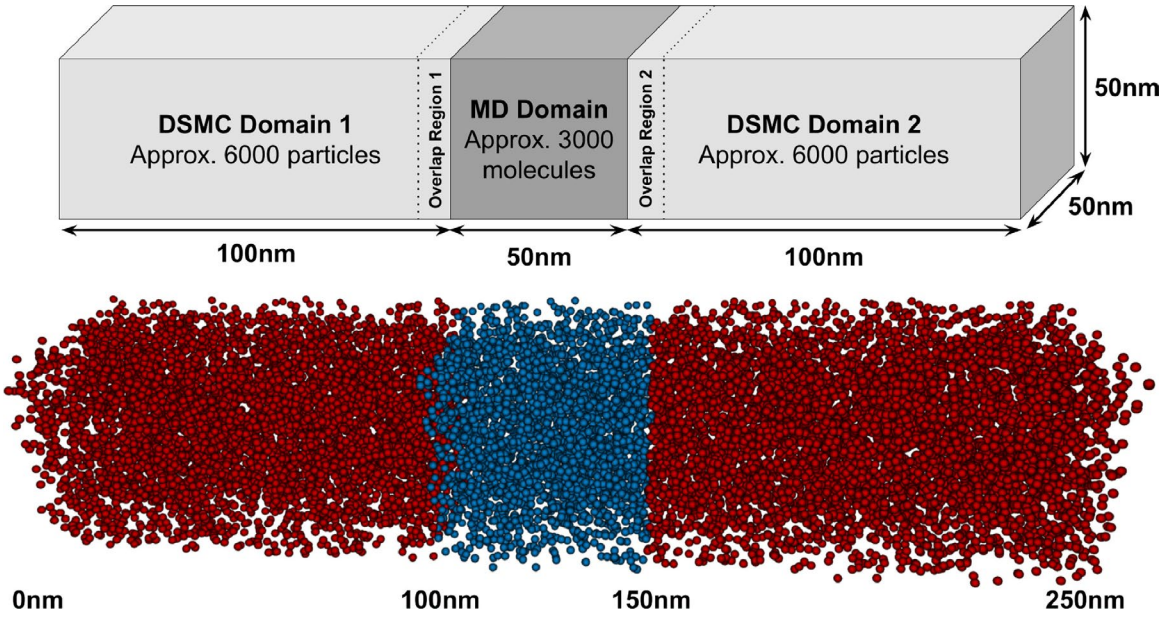
openfoam.com

The Benefits

By enabling OpenFOAM-based solvers to connect directly with numerical frameworks through MUI, users can now perform multi-physics and multi-scale simulations. It simplifies intricate coupling workflows, removes the need for manual code adaptation, and allows simulations to be built, tested, and deployed efficiently across modern high-performance computing systems.

The convenient use of MUI in OpenFOAM has already facilitated a new code structure known as a ParaSiF (Parallel Partitioned Simulation Framework), which enables OpenFOAM to couple with other specialist solvers to capture complex interactions. This new code structure not only makes it effortless to expand and meet the needs of different users but also can be easily maintained in the long run.

All codes used are of an open-source, community-oriented design that aligns with CoSeC's mission to make advanced computing accessible across disciplines. It empowers researchers from diverse backgrounds to construct high-/multi-fidelity coupled simulations without the steep learning curve traditionally associated with high-performance computing.



MUI enabled Molecular Dynamics to direct simulation Monte Carlo coupling

Image credit: S. Longshaw, R. Pillai, L. Gibelli, D. Emerson, D. Lockerby, Coupling molecular dynamics and direct simulation monte carlo using a general and high-performance code coupling library, Computers & Fluids 213 (2020) 104726.

Next steps

This new capability with ParaSIF is now being applied to the simulation of floating offshore wind turbine systems, where accurate modelling of coupled fluid–structure dynamics is essential to improve performance, safety, and resilience. Beyond renewable energy, this same approach will benefit not only the WSI community but also wider communities studying coastal and marine engineering applications.

By enabling codes like OpenFOAM and other widely used solvers to work together seamlessly, CCP-WSI and MUI are helping to build a stronger, more connected research ecosystem capable of tackling the next generation of multi-physics and multi-scale challenges.

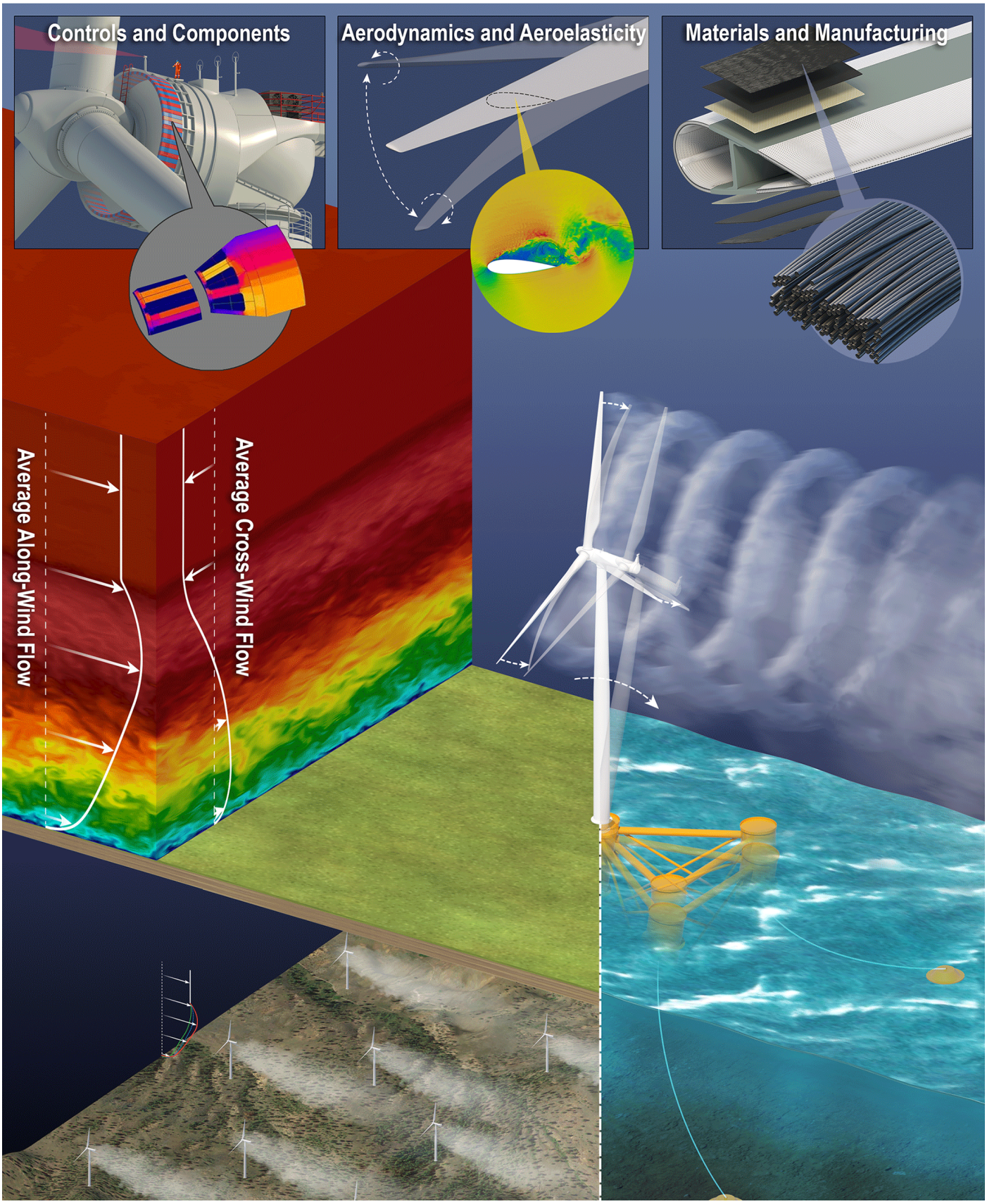
"By lowering the technical barriers, researchers are now able to focus on scientific and engineering insight rather than software integration. We are now supporting a growing ecosystem of advanced applications. As well as wave–structure interaction simulations for offshore and coastal engineering, we are now working on machine learning simulations, where models are integrated directly into physics-based solvers, developing heat transfer modelling for cryogenic systems, which is critical in low-carbon aviation and maritime transport."

Wendi Liu

CoSeC Project Lead for CCP-WSI, STFC Scientific Computing

Read more about Parallel Partitioned Simulation Framework

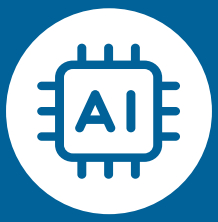
github.com/ParaSiF


Controls and Components
Aerodynamics and Aeroelasticity
Materials and Manufacturing
Average Along-Wind Flow
Average Cross-Wind Flow

Metrics

Research Software as a National Infrastructure

Technical



Applied AI

Accelerated Computing

Quantum

FAIR

Energy Efficiency

Community

Training

Software Maintenance

Coordination

RTP Careers

Metrics

52
Publications

90
Presentations

4916
Training Days

66

4395
Citations

Continued development and launch of the CoSeC Catalogue will help to ensure the application of FAIR principles.

The CoSeC Energy Efficient Computing Project will identify common challenges related to energy efficient computing in line with challenges identified by a number of communities[1] and develop follow-on projects to determine best practice.

Development of online training platforms with multiple communities and using various platforms[2], alongside continued investment in training courses, summer schools and workshops will make CoSeC training accessible to more people and communities.

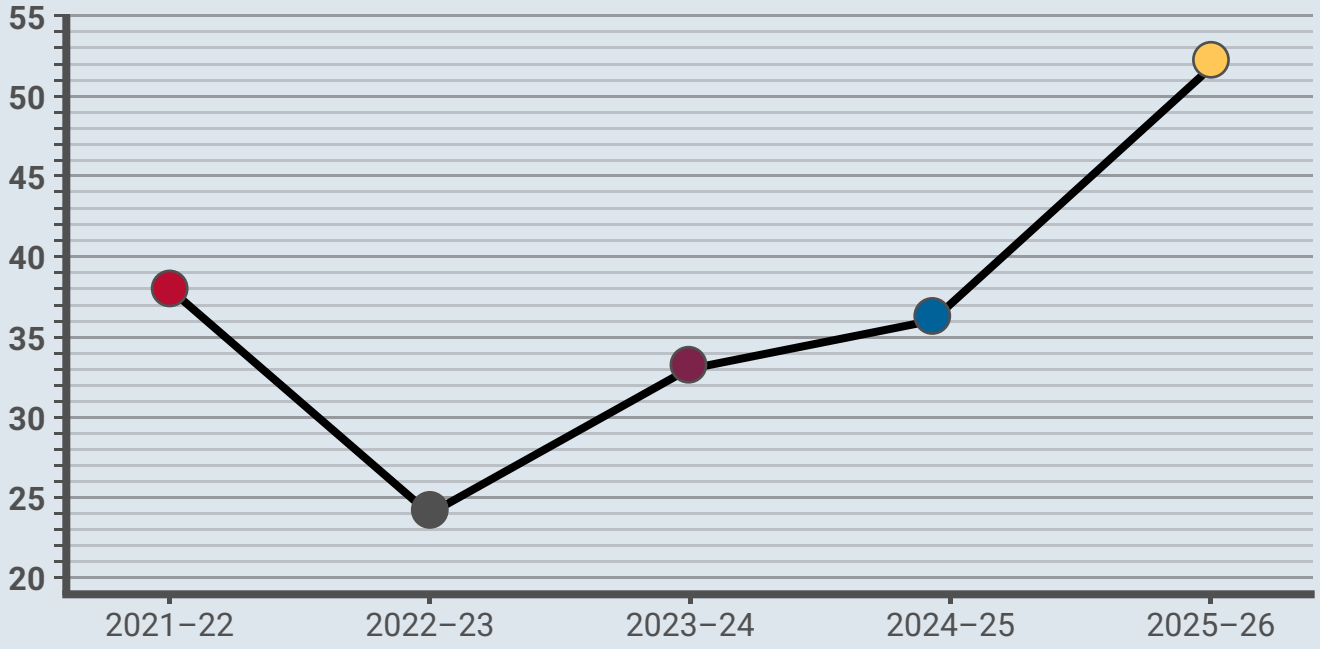
The CoSeC Fellowship Programme will continue to help identify and develop RTP careers via training opportunities, knowledge exchange and exposure to new technology.

Interaction with the NPRAISE Programme will offer exciting upskilling opportunities in AI.

52
Publications

Generating impactful publications with our colleagues from the CoSeC communities

Publications Between 2021–26

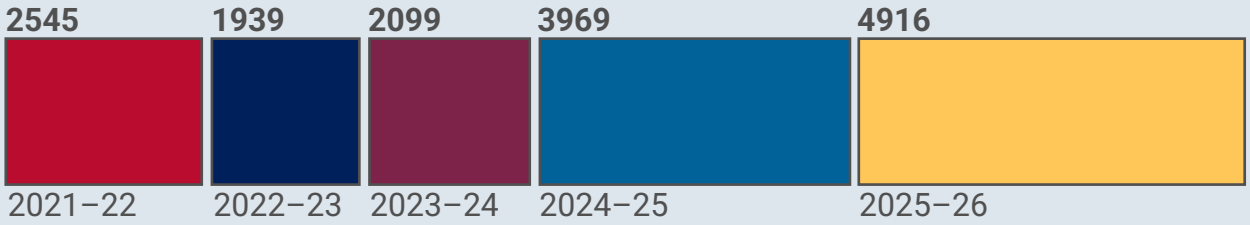


1 and 2. CoSeC 2025 Mid-Year Forum Report (DOI: 10.5286/stfcconf.2025002) and CoSeC 2025 Year-End Forum Report (DOI: 10.5286/stfcconf.2026001) cosec.ac.uk/calendar/cosec-community-forum/

4916
Training Days

Generating impactful publications with our colleagues from the CoSeC communities

Training Days Between 2021–26



Online Training

Making training more accessible!
The number of online courses now available through communities has increased by more than 50% with over 40,000 views of some training courses.

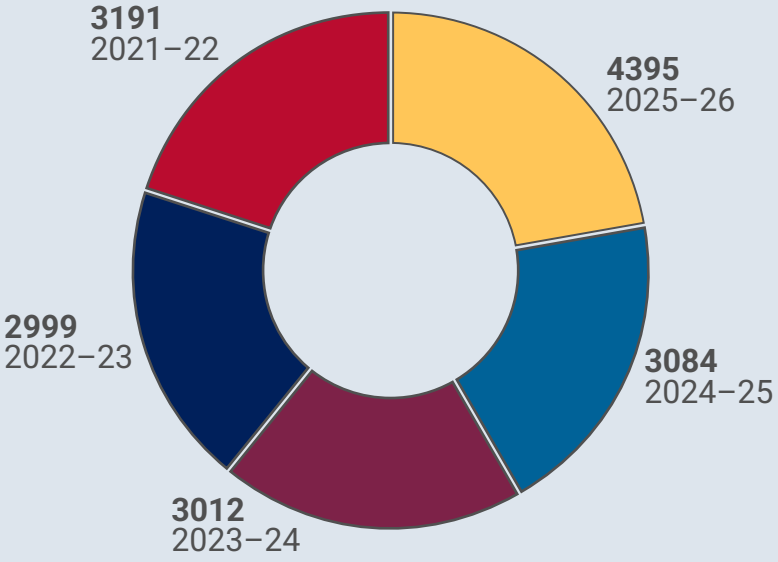
Academic Licenses

Making software more accessible!
Academic group licenses and downloads for community codes like CASTEP continue to rise with almost 2400 groups currently making use of the CASTEP software.

4395
Citations

Enabling the creation of papers, reports and publications through work using our codes

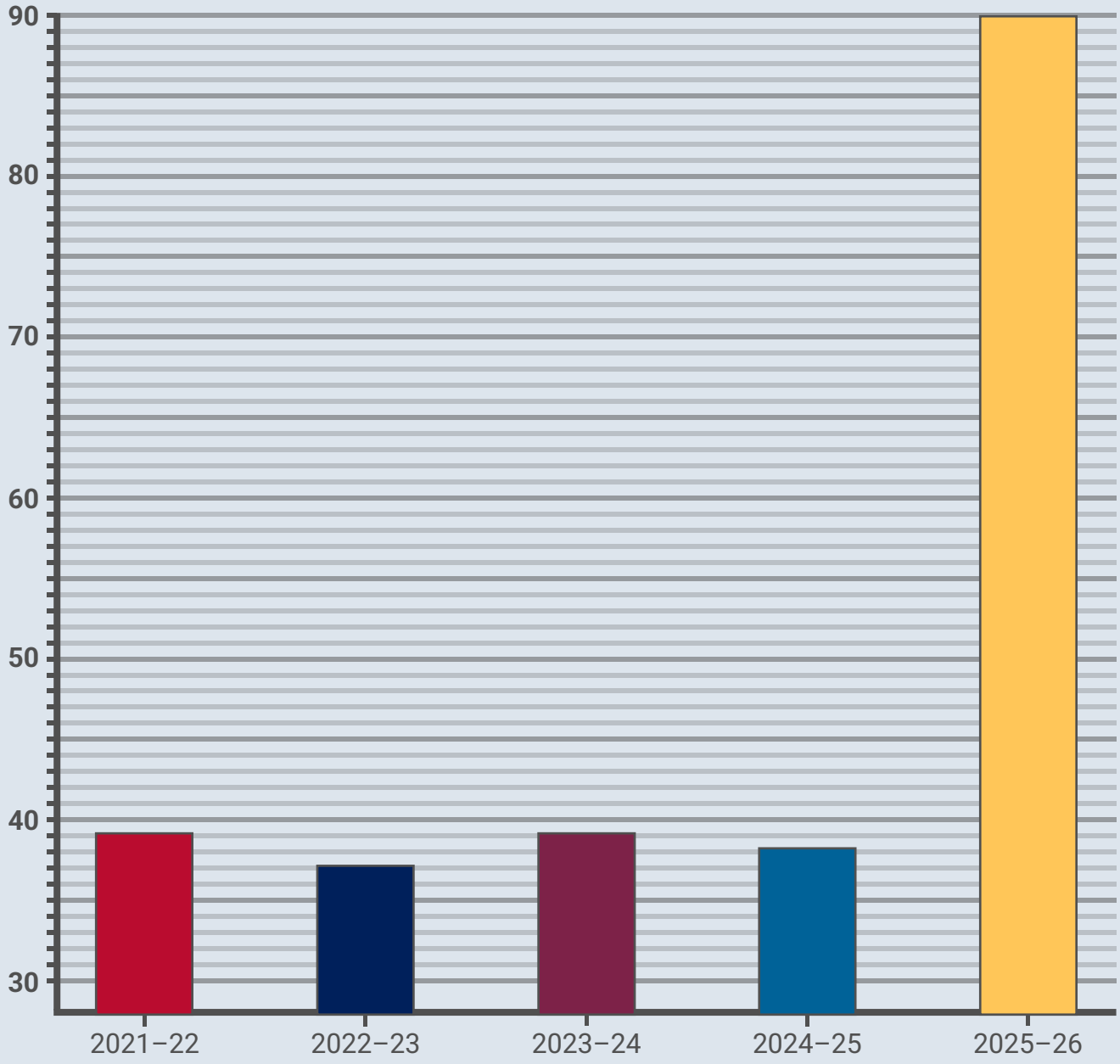
Citations Between 2021–26



90
Presentations

Engaging with the communities and more by presenting CoSeC work to a wider audience

Presentations Between 2021–26



Expanding CoSeC Communities

Enabling the creation of development of new communities in different scientific fields.
Funding six new communities to expand the remit of CoSeC and encourage engagement from different scientific areas.

Testimonials

“You would never be able to do anything like building our CCPBioSim platform without CoSeC. The fact is that we can organise academics across the country to create material for a common purpose – in this case, upskilling. Today scientists are trained more in laboratory conditions, rather than in computing, so they need to be trained in these skills. Every university has to train their own scientists, and we have the capability, expertise and technology to deliver the training and enable them to quickly move forward together.”

James Gebbie-Rayet

CoSeC Project Lead for CCPBioSim, STFC Scientific Computing

“What I enjoyed most about being a CoSeC Fellow was the opportunity to take on a meaningful role that allowed me to grow both professionally and personally. The Fellowship gave me the confidence to engage more actively in networking at different events which was valuable for broadening my professional connections. With the support of the Fellowship, I had the chance to attend two conferences, including a major international conference on transport research, where I presented our latest research progress and received constructive feedback. The Fellowship encouraged me to take initiative in expanding my professional network and engaging with peers and mentors in ways that I might not have otherwise.”

Qian Fu

CoSeC 2024 Fellow

“CoSeC provides a central pool of expertise to help with both practical project-management and communication. By bringing together different research communities under one roof, it’s much easier to see how value can be added, e.g. via small tweaks to a workplan means a tool can support more than one community at the same time, or where joint training would make sense. CoSeC also provides funding and steering, allowing communities to continue to push the boundaries of cutting-edge research whilst aligning with national objectives.”

Kane Shenton

CoSeC Project Lead for CCP-NC, STFC Scientific Computing

“The aspect I appreciated most was the Fellowship’s intent to provide flexible support and visibility within the CoSeC community. The funding itself was helpful in principle, and the Fellowship has clear potential to be a strong mechanism for supporting researchers across computational science with more structured engagement in future iterations.”

Christian Gutschow

CoSeC 2024 Fellow

“The Fellowship was a launchpad for my research and enabled work that matters and relationships that last. I look forward to continued collaboration with CoSeC.”

Ignatius Ezeani

CoSeC 2024 Fellow

“There is a great deal of knowledge that is curated and passed on from the CoSeC communities that has helped us make these essential connections. Colleagues at CoSeC have enjoyed being part of the research and therefore, they are like equals with us in the work that we do, which has been great.”

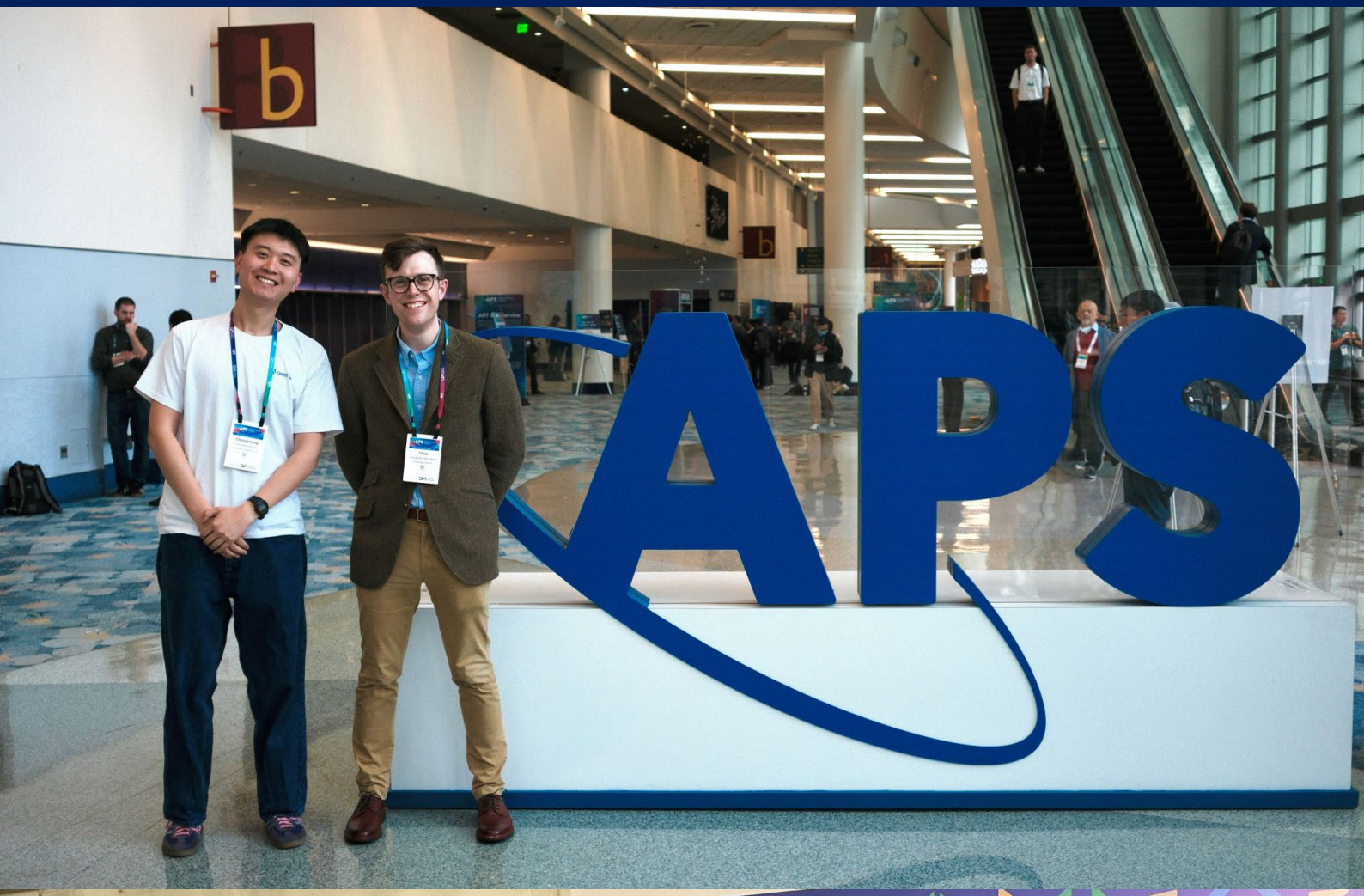
Professor Viv Kendon

CCP-QC Chair

“Working with CoSeC has enabled CCPBioSim to build a coherent and long term community that is internationally recognisable, and strongly valued. CoSeC helps us with vital infrastructure such as our website, mailing lists and provides a repository for our training materials and software. CoSeC supports our organisation of online and in-person conferences, training workshops and seminars. For example, our monthly industry seminar series has been running since 2020 and is supported by CoSeC, regularly attracts over 50 attendees, has speakers booked through until the summer of 2027. CoSeC has also provided us with industry-standard technical expertise in software development, enabling us to support and develop computational methods that the community would otherwise have lost, such as our flagship CodeEntropy software. Consistent and reliable provision of support and expertise is vital in a research environment where most grants are short term, because much computational research infrastructure is only valuable when it can be confidently maintained. CoSeC is also important in maintaining connections to other DRI initiatives such as the PSDI. This helps build connectivity within DRI infrastructure provision, which is essential for it to be of most value to UKRI. ”

Sarah Harris

CCPBioSim Chair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Scientific Computing