Computational Science Centre for Research Communities

Financial Year 2022-2023 Annual Report

(*Covering the period 1 April 2022 – 31 March 2023*)

Report Submitted June 2023

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1. Executive Summary 2022-23

EPSRC HEC renewal call: the outcome of this has evolved the landscape of the communities supported by CoSeC. The CoSeC support now concentrates on the four main areas of material science, computational engineering, biological sciences and tomographic imaging. The area of atomic, molecular and optical physics, and the area of plasma physics, are no longer supported directly by CoSeC. The current number of EPSRC communities supported is 15.

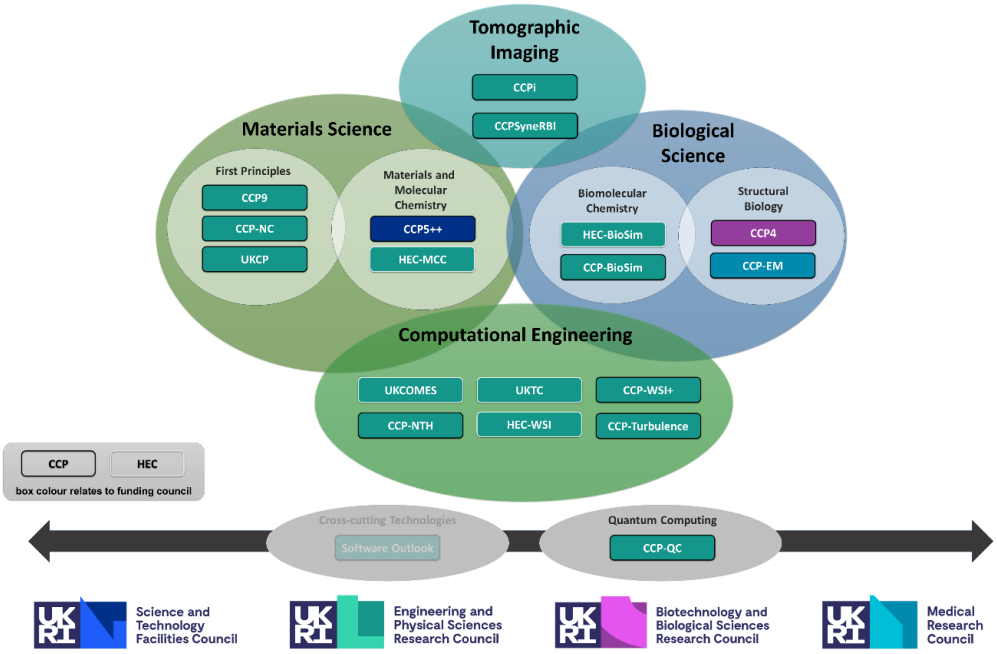


FIGURE 1: COSEC LANDSCAPE (AFTER 2022 HEC RENEWAL)

Reset of EPSRC-CoSeC FTE allocation: as described in Section 4 EPSRC has changed the allocations of CoSeC effort to the EPSRC-funded communities in order to resolve the issue of the mismatch between CoSeC resources allocated to the communities and funding given to CoSeC. In their reports for the June 2023 CCP Steering Panel meeting, the communities Chairs have stressed that the reductions are going to impact the sustainability of their software, the ability to deliver training, coordinate networking events, disseminate their impact and make efficient use of research infrastructure such as the National Supercomputing Facility ARCHER2. While these consequences are lamentable, CoSeC leadership would like to thank EPSRC's Elizabeth Bent for addressing the issue of this mismatch, which was causing the progressive widening of a gap between the level of resources the communities expected, and what CoSeC could afford to deliver within the budget allocated.

Large scale computing: In FY2022/23, working synergistically with other investments such as the ExCALIBUR and EPCC's eCSE programmes, CoSeC has delivered significant advancements in software for large scale computing.

CoSeC support for CCP9 and MCC, in collaboration with activities funded by the ExCALIBUR programme and international academics, have delivered a new version of the CRYSTAL code, a powerful and scalable computational tool for solid state chemistry and physics. The new code includes yet more powerful parallelism features for high performance computing, and is now available on ARCHER2. The version release was accompanied by a peer-reviewed publication about the code, which was chosen as a highlight by the APS Journal Editor.

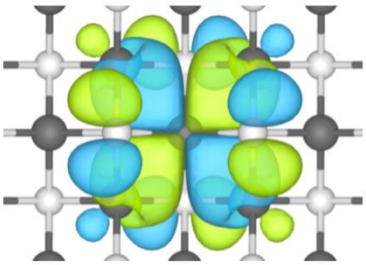
Py-ChemShell the scalable software for multiscale computational chemistry developed for the MCC, is also now available to all ARCHER2 users. Py-ChemShell has been interfaced to the basis set library by the US initiative MolSSI, via its standardised API, offering a simple and flexible way to select basis sets in quantum-mechanical calculations.

Various CCPs and HECs in the Computational Engineering space are directly involved in large scale computing initiatives. For example, the Xcompact3d software (which is significant for the UKTC and CCP-Turbulence communities) and the general-purpose code coupling library the Multiscale Universal Interface (which underpins activities within the CCP-WSI+ and HEC-WSI communities), are both directly included in the EPSRC funded part of the ExCALIBUR programme. These software packages are also being developed as part of an ongoing Intel funded Centre of Excellence operated by CoSeC staff looking at the application of heterogenous programming.

Considerable work has been invested in supporting new HEC Biosim users getting set up and running on ARCHER2, and the Tier2 systems JADE2 and Bede. Also, the online application structure for obtaining time on ARCHER2 and the Tier2s via this consortium has undergone a radical improvement. The CoSeC support for the resource allocation panels (RAPs) now focusses on the technical assessment of scientific cases against the resource requests, and studies are now automatically placed upon the optimal high-performance computing (HPC) resource based on benchmarking and specialist expertise.

Data Infrastructure: CoSeC has worked synergistically with data-infrastructure initiatives. Examples are collaborations that have been established between the Physical Sciences Data infrastructure (PSDI) and:

- The bio-simulation communities, to seamlessly integrate process recording into the research workflow, by creating a plugin to the existing software AiiDA, and a user environmental prototype. This project is being extended to provide simulated cryo-EM data that will be of great use to the CCP-EM community.
- CCP-NC, where a joint appointment has been made to expand and integrate the database of simulated solid-state NMR parameters into PSDI, for long-term curation and maintenance and linkage with other data sources.
- The Computational Materials Science communities, to create a database and associated tools for generating machine-learned interatomic potentials from first principles data, towards trusted AI-enabled research.



Software: In collaboration with Imperial College London and Oxford University, a CoSeC team across the support for CCP9, MCC and UK-AMOR communities have completed a drastic revamp of the Wannier90 code. This software enables the calculation of advanced electronic properties of materials with high efficiency and accuracy, and is interfaced to many of the most popular electronic structure codes. Workflow, readability, and functionality have all been drastically improved with this new version. This major milestone has been committed to the public repository and is currently in pre-release testing mode.

The CASTEP user base (supported by CoSeC via UKCP, MCC, CCP-NC and CCP9) continues to grow rapidly, with an additional 411 groups obtaining an academic licence during 2022/23. This has been enormously facilitated by the introduction of a world-wide cost-free source-code academic license for the code (see Metrics section for overall figures).

Thanks to the CoSeC support for CCPBiosim, the existing codes for calculating the entropy of proteins and solvent have been brought together with CodeEntropy. The project has been successfully completed and the code has been released on GitHub.

Work within CCP-NTH has seen a core simulation code CHAPSim redeveloped and released over recent years, recently the 2decomp&fft pencil-decomposition library has been integrated into the code, allowing significantly better scalability for certain simulations. This work is in conjunction with UKTC and CCP-Turbulence, where 2decomp&fft is utilised within other community codes, this has seen the library developed into its own stand-alone repository with modern build system and GPU offload and released for general use.

The CoSeC team that supports CCPi and CCP SyneRBI have collaborated closely with UK and international large experimental facilities on the Core Imaging Library (CIL). This has been possible thanks to the synergy with the STFC Scientific Computing initiative in support of large Facilities science – the Ada Lovelace Centre. In collaboration with the UK neutron and muon source ISIS, they have worked to provide CIL powered iterative reconstruction and algorithm improvements. With the European Synchrotron Radiation Facility beamline I19 they have provided a standard CT reconstruction pipeline, with the development of a new ad-hoc reader.

The CIL developers team participated in the Helsinki Tomography Challenge, an open challenge organised by the Finnish Inverse Problems Society on limited-angle computed tomography. Their algorithm developed in CIL, granted the team 3rd place in the competition.

A case study was produced for the DL_MESO code, provided by CoSeC in support of the UK COMES community, and is included below.

Training: The CCP Biosim on-line training platform has had a major completed rebuilt, and migrated to STFC hosted harbour due to sun-setting of free tier access. This has resulted in an improved speed of the service. The metrics have also been expanded for training notebooks, so that CCPBiosim can now get access to a very advanced set of telemetrics about how their on-line training resources are used.

A joint hackathon with CCP SyneRBI and PET++, took place with the aim to establish a suitable reconstruction evaluation strategy, including metrics for image quality and algorithm performance (run-time, memory etc.), taking into account parameter selection for algorithms used. This will lead to an open framework for evaluation of image reconstruction algorithms.

A Hackathon was also held for the new software CodeEntropy in order to improve its functionality and user friendliness.

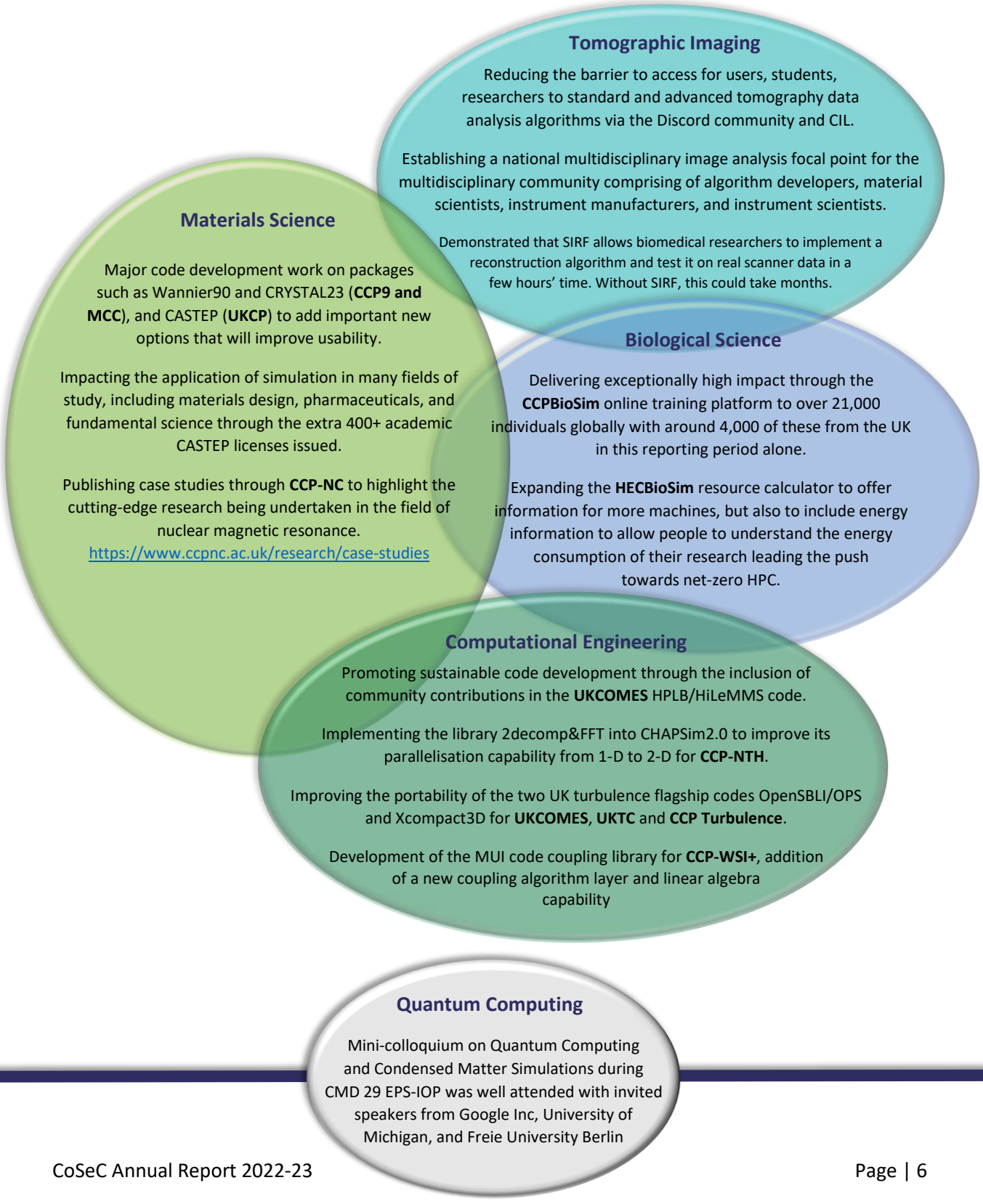
Community building and coordination: A new software strategy has been created for the CCP WSI+ community in consultation with the University of Plymouth. This will be reviewed, refined and actioned over the FY2023/24. This aims to formalise all of the ongoing threads of activity wrapped up in WP1 and WP2 of the current CCP WSI+ grant, and present a picture of how it all fits against a key problem type for the WSI community: the floating offshore wind turbine.

Considerable CoSeC effort has been invested in the CCP-NC community building activites. A quarterly online discussion meeting series covering topics relevant to computational solid-state NMR was set up. In addition, a travel fund for early career researchers was launched, as well as an international engagement fellowship scheme to help promote interactions following the COVID19-related restrictions. The result of this community building effort is paying off, with the number of active subscribers to the CCP-NC mailing list doubling since 2021.

CoSeC support helped deliver a number of new websites, including the one for CCP9 and CCPBiosim. On the CoSeC website, the list of blogs contributed by CoSeC staff is growing steadily: https://www.scd.stfc.ac.uk/Pages/CoSeC_blog.aspx.

2. Impact 2022-23

In this section we highlight some areas where the work of CoSeC during this reporting period (1 April 2022 – 31 March 2023) is having an impact in our communities, across our communities and further into the general public domain.



Efficiently and discretely modelling shallow water flows

CoSeC
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Natural disasters involving flow such as flooding and tsunamis often lead to a loss of lives and considerable economic damage. For example, in 1993 a tsunami generated by a magnitude-7.8 earthquake inundated Okushiri, Japan causing the death of 165 people; in the UK flooding causes £1.3 billion of economic loss each year[1]. Understanding these flows is a crucial step towards mitigating their devastation, and the application of computational modelling techniques is one important method contributing to this field of research.

Dr. Jianping Meng, Dr. Xiaojun Gu, and Prof. David Emerson, (computational engineers at the Science and Technologies Facilities Council (STFC)) Mr Yunlong Fei, Dr. Peng Yong*, and Prof. Jianmin Zhang (at the State Key Laboratory of Hydraulics and Mountain River Engineering (SKLH), Sichuan University, China) developed software to simulate realistic flow problems such as a tsunami inundation.

1993 Hokkaido earthquake and tsunami: Aonae, Okushiri Island, looking southeast. Structures in the foreground were damaged by fires fueled by above-ground kerosene and propane tanks following the tsunami. The concrete steps provided a means of escape for some residents following the strong earthquake[2]

Enhancing the lattice Boltzmann method

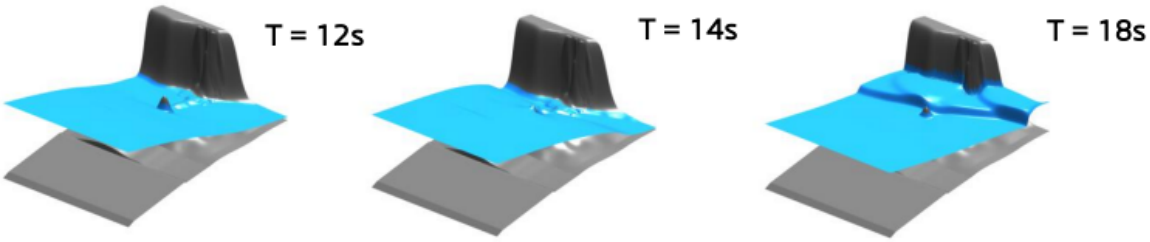
The lattice Boltzmann method (LBM) has emerged as an easy-to-understand modelling tool for fluid flows. Rooted in the kinetic theory of gases - where identical particles move in random directions – the LBM is formed by discretizing the statistical Boltzmann equation on a grid ('lattice'). Although used in the shallow water model, LBM needed further development to make it applicable to supercritical flows that occur in natural disasters[3]. To simulate these more realistic problems, e.g., tsunami inundation, it is necessary to model the drying-wetting interface that is moving during the inundation. 'Vanilla' LBM lacked this capability, and was in need of development.

[1] Flood risk and the UK Energy & Climate Intelligence Unit
eciu.net/analysis/briefings/climate-impacts/flood-risk-and-the-uk

[2] National Centers for Environmental Information
ngdc.noaa.gov/hazardimages/#/all/46

Discrete Boltzmann model (DBM)

To tackle this challenge, the team developed a type of discrete Boltzmann model (DBM) by applying a specific type of polynomial expansion i.e., the Hermite expansion approach[3] to the LBM. This extended the model's capability to supercritical flows without much loss in efficiency and simplicity. The model was then implemented into the multiple platform lattice Boltzmann (MPLB) code within STFC's general purpose mesoscale simulation package - DL-MESO.



High-resolution snapshots of a discrete Boltzmann model (DBM) simulation of a tsunami run-up onto a complex beach profile showing the 3D water height distributions at different times, (T). Grey denotes the sea bathymetry (surface of the underwater floors); and blue is the height of the surface of the water.

To simulate the drying-wetting phenomenon seen, for example, in a tsunami inundation the research team implemented various schemes based on the MPLB code and tested them over a range of benchmark problems. In particular, they compared the DBM simulations with the experimental data produced using a large-scale tank for exploring the extreme run-up of 32m height observed near the village of Monai during the 1993 Okushiri tsunami[4]. The computer simulations were conducted to model a sub-region of the tank where there are complex bathymetry (underwater floor surface profiles) and coastal topography. Preliminary testing demonstrated promising results, confirming the successful implementation and application of the MPLB code to such shallow water flows.

How to obtain DL-MESO

Follow the instructions on this page to register:
https://www.scd.stfc.ac.uk/Pages/DL_MESO-register.aspx
Then follow the instructions that are emailed to you on successful registration.
DL_MESO is one of the software codes developed by **UKCOMES** (ucl.ac.uk/mesoscale-modelling-consortium) that is one of the 19 communities supported by STFC scientists and engineers through the CoSeC project (cosec.stfc.ac.uk)

[3]Meng JP, Gu XJ, Emerson DR, Peng Y, Zhang JM (2018), Discrete Boltzmann model of shallow water equations with polynomial equilibria, International Journal of Modern Physics C 29: 1850080-15; [4]Liu P. L.-F, Yeh H, Synolakis C (Eds.), Advanced numerical models for simulating tsunami waves and run-up, Vol. 10. World Scientific, 2008.

Funding: This work was sponsored by: The Royal Society – 2015 China (NSFC) Cost share programme; UK Consortium on Mesoscale Engineering Sciences (UKCOMES, EP/R029598/1). This work used the ARCHER UK National Supercomputing Service (http://www.archer.ac.uk). The Computational Science Centre for Research Communities (CoSeC) (cosec.stfc.ac.uk) provided STFC staff support. **Further Information**:*Dr. Yong Peng's present address -School of Natural and Built Environment, Environmental Change and Resilience, Queens' University Belfast (https://pure.qub.ac.uk/en/organisations/school-of-natural-and-built-environment)
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archer

Not one but two joint winners of the 2022 CoSeC Impact Award

Now in its third year, the CoSeC Impact Award was launched in 2020 with three main aims: to be a means of recognising the work of researchers early in their careers who have been, or continue to be, supported by CoSeC; to be a means of raising the awareness of the communities supported through CoSeC1; and to be a means of acquiring evidence of the impact of CoSeC and the communities it supports in science.

Thanks again to the generous support of NAG (the Numerical Algorithms Group) the prizes include vouchers to the value of £250 for this year's two joint winners: **Claire Delplancke and Catherine Disney** - Congratulations!

Dr. Claire Delplancke (Research Associate in the Department of Mathematical Sciences, University of Bath)

"As an applied mathematician, I work on translational research from the Imaging Science field to the Medical Imaging field, with a focus on Positron Emission Tomography (PET). PET is a functional imagery technique which permits to reconstruct a map of activity in the body, making it relevant for the detection of tumours. The goal of my research, which relies on open-source software from CCP SyneRBI[2] and CCP Tomographic Imaging[3], is to bring advanced reconstruction algorithms from the Imaging Science field to PET clinical practitioners. Down the line, we hope to improve the diagnosis of tumours in cases which are difficult to diagnose with the current techniques, and to localise them more precisely in order to guide surgery. In the next step of my career, I'll join an international electricity company and focus on energy mix optimization."

Dr. Catherine Disney (Research Fellow in the Department of Mechanical Engineering at University College London)

"My research has been to develop *in situ* x-ray tomography imaging and digital volume correlation (DVC) processing methods to meet the specific needs of tissue biomechanics. DVC is fundamental in the quantitative interpretation of tomography-based *in situ* experimentation, enabling the measurement of nanoscale strains within intact samples. Such measurements are valuable in quantifying tissue biomechanics since tissue mechanical function is profoundly dependent on microstructural dynamics and mechanobiology-driven pathology occurs within the nanoscale environment. My work has focused on quantifying intervertebral disc microstructural dynamics of collagen fibres using *in situ* imaging and DVC.

In the future, I would like to lead my own research team and continue developing microstructural-based DVC analysis for tissue biomechanics. My future hopes are to collaborate with mechanobiology groups in applying these methods to investigate disease and degeneration models of soft tissues and to assess the efficacy of new treatments. There are also some exciting challenges ahead for DVC analysis as the next generation of extremely brilliant source synchrotron tomography beamlines emerge, providing scope for larger samples and shorter scan times, paving the way towards more clinically relevant dynamic studies. Finally, I look forward to continuing working with CCPi[3] staff to further develop functionality of the iDVC app and help train future users."

3. Outline Plans 2023-24

This section contains the individual outline plans for 2023-24 for the CoSeC supported CCPs and HECs.

Materials Science

CCP9

The spin-orbit and GPU porting work on ONETEP will be one of the major tasks during this period. Possibly optimizing CASINO will be part of the CCP9 plans should this be decided to go ahead with Neil Drummond at Lancaster University. Compton profiles collaboration with Bristol will be part of the CCP9 plans should this be decided to go ahead. Both activities would stretch into 2024.

CCPNC

Following our expansion of user engagement activities (WP2.1–WP2.3), we will continue to run the CCP-NC Online meeting series. Planning is also underway for a Faraday Discussion meeting on NMR Crystallography (now approved) and, separately, for a joint meeting with CCP5 and CCP9. Further, an industrial engagement post-doctoral research assistant has started this year and will provide a valuable link to partners in the pharmaceutical industry.

Maintenance and expansion of core tools: MagresView 2.0 (WP1.1a) and Soprano will form a significant part of our planned activities in the coming year. In addition, we will be releasing the new code to tackle disorder in organic crystals as part of work packages WP1.1b and WP1.3a.

Finally, recruiting is underway for a person dedicated to the Magres database (WP1.2) redevelopment. Their tentative start date will be August 2023. This will be a joint position with the Physical Sciences Data Infrastructure (PSDI) initiative and will include efforts to improve the interoperability of the Magres database with other materials databases in accordance with the FAIR data principles.

UKCP

In direct support of the UKCP and wider CASTEP community, the annual CASTEP software release management, teaching workshop and code developer's workshop will be carried out. Maintenance of the software development and testing platform will allow for the continued growth of the CASTEP package and the software standards required and expected by the commercial partners and academic community.

We will build on the success of the electronic licensing for CASTEP to provide a simple and secure mechanism for HPC administration teams to verify if a user has an active user licence. This will reduce day-to-day workload on CoSeC staff in favour of code and method development activities. It will also reduce the time for licenced academic CASTEP users to be granted access to centrally installed versions of CASTEP on services such as ARCHER2.

A three person-month project will be carried out to quantify the errors from a commonly used approximation in hybrid-DFT calculations in simulations that make use of pseudopotential representation of atomic core electrons. This will inform users of the limits and accuracy for existing workflows and provide guidance for future method and code development in this area.

MCC

The MCC CoSeC workplan for 23/24 is the first to be based on the CoSeC proposals for the new HEC cycle, with initial priorities identified under the three work packages of ab initio DFT, classical/ML forcefields and multiscale methods. Ab initio DFT support is currently focussed on optimising CRYSTAL23 for the upgraded ARCHER2 service. The classical MD theme has been widened in the new cycle to include support for improving accessibility to ML methods for interatomic potentials, with an

initial assessment underway for MOFs. For DL_POLY, engagement with the MCC community is a key priority through the holding of a community workshop, while DL_FIELD will be improved through with support for a wider range of file formats and materials forcefields, to be included in v4.10. Support for multiscale QM/MM methods will include rigorous testing and benchmarking ChemShell on ARCHER2 following the programming environment upgrade, extension of the new subtractive QM/MM functionality to materials systems with a periodic description of the environment, accessibility improvements through integration of automated zeolite FF management via DL_FIELD, and integration of machine learning accelerated optimisation methods into the public release of the DL-FIND geometry optimiser.

Due to limited staff availability at present, especially for ab initio DFT support, the provided 23/24 workplan reflects a reduced total effort of 1.1 FTE. We anticipate that this will rise to the allocated 2.1 FTE following recruitments in this reporting period, and additional tasks will then be added to the plan as appropriate, in discussion with the MCC community.

Biological Science

CCPBioSim

In 2023/24, CCPBioSim will continue with our regular schedule of training, conferences, and industry talks. We will also work on short (6-12 months) software projects including implementing finite temperature string methods for enhanced sampling into Plumed. There will be new short software projects announced in the next reporting period, but these are currently in the application pipeline and have to go through CCP management committee approval.

HECBioSim

The 2023/24 plans are in an early stage of planning due to the ongoing renewal process for the HEC consortia. The plans for the 23/24 year will contain a large element of ongoing support for the consortium and its researcher users with activities relating to running biomolecular simulations across UK HPC resources. The community would like to see more HPC focused training, so we will develop a series of HPC focused course for biomolecular simulation. The platform behind the HEC website reaches end of life in summer 2023 so a new website will be required so a branding and content refresh will occur in tandem. We will expand the benchmarking suite, both in terms of the codes that we will test and also the types of benchmarks we are doing will be expanded significantly to allow researchers to understand how the types of simulations within a particular code affects resource requirements and energy usage.

Computational Engineering

UK-COMES

Interfaces in both the DPD and LBE codes of DL_MESO based on HiLeMMS will be created to couple both methods together and enable hybrid multiscale modelling along similar lines to previous approaches involving atomistic molecular dynamics and computational fluid dynamics. The connection of molecular modelling (DPD) to larger-scale hydrodynamics (LBE) will enable more accurate simulations of systems where both phenomena are important, e.g. plasmid solutions undergoing electric fields.

The major work for the HiLeMMS domain-specific language will be to enhance the integration of the AMReX code for an adaptive mesh refinement (AMR) capability and to test the code for a range of problems. This will greatly enhance the capability of the LBE method to simulate multi-scale real-world flow problems.

CCP-WSI+

The design challenge of how to create a general-purpose, extensible and open-source multi-physics framework for the WSI community has been a grand challenge task since before CCP-WSI+ began and also provides the driver for technical work to be undertaken in the new HEC-WSI community in future reporting periods. Primarily, the goal is to create a framework that can be extended by somebody else in the WSI community other than the main developers in order to add a new solver to the framework to augment its physical capability. This is no mean feat in software terms but with the plan in place for 23/24, the ParaSiF framework (plus solver capabilities from the WSI community) will become a good starting point.

Addition of new coupling algorithm capability to MUI will ensure that new couplings can be created following examples, this will be supported by a "quick start" style guide to complement the existing Doxygen generated documentation that comes with the library. The conclusive tasks for this CCP will focus on data workflows between solvers in order to create a truly cohesive framework for use by the WSI community going into the future.

Tasks around improving performance of coupled solutions through dynamic load balancing will automatically be able to be incorporated into the OpenFOAM-based elements of ParaSiF and the MUI library itself is being performance engineered through a number of ongoing projects within STFC.

The creation of a new Research Object catalogue is a great outcome for the CoSeC support of this community and a new and interesting initiative for software data collation, it has great potential for use across most CCPs and HECs and will be championed by the CoSeC project management office once it is in the public domain.

HEC-WSI

The High End Consortia for Wave Structure Interaction (HEC-WSI) was created to address the issue that while the WSI community has a significant number of highly complex and challenging modelling and simulation problems, its use of high-performance computing is currently too limited in scope. This is particularly evident in that a large amount of the communities computational science is driven by the OpenFOAM package but knowledge of how to best use this on supercomputing resources like ARCHER2 is misunderstood and underdeveloped. Many problems that could scale to significant portions of the machine are instead tackled at lower fidelities on moderate workstations. This HEC will address this through community education and guidance, direct development of software and by providing provision and access to HPC where it didn't previously exist.

Another aspect of HEC-WSI is that the corresponding CCP-WSI+ community has identified large-scale multi-physics code coupling as a core driver, this effectively means created simultaneous partitioned workflows to enable the simulation of complex problems like floating offshore wind turbines (FOWT). Code coupling at scale on the likes of ARCHER2 is non-trivial, with the need for direct support and development of software, as well as methods. The CCP-WSI+ CoSeC workplan is directly tackling the creation of working software to handle FOWT-like problems, this includes fully coupled solutions involving multiple open-source solvers to tackle different aspects of the physics of the problem, as well as general purpose coupling capability in the form of the Multiscale Universal Interface library. The HEC-WSI will support this work by exploring and developing aspects like the scalability of the MUI library on ARCHER2 for problems related to WSI and benchmarking and development of the components of the coupled solutions (e.g. the OpenFOAM based interFoam CFD solver or CoSeC's FEniCS based structural solver).

The HEC will also consider how computational science related to WSI should advance, taking into account the clear directions of supercomputing, such as the shift towards heterogenous compute involving GPUs, ensuring that work done by the WSI community is well aligned with the most likely HPC trends for the UK in the coming years. Examples here include integrating, understanding and disseminating the key outputs from major work happening to important codes (e.g. the exaFOAM EU H2020 project looking to port OpenFOAM to GPUs and improve its scalability) as well as benchmarking and directly developing the communities own solvers and codes.

Finally, in direct collaboration with the RSE support provided at Plymouth University, the CoSeC support for HEC-WSI will work on developing scientific drivers and use cases to highlight he need for large-scale HPC within the community.

As this community has both a CCP and HEC activity and both are very closely aligned, it is the intention moving forwards to ensure that the work done by CoSeC across both activities is shared wherever possible, this means that while both projects retain a level of independence, the overall workplan for both will undoubtedly have overlaps in places. This is seen as a good use of CoSeC resources and a sensible way to cross-cut.

CCP-NTH

The main community building and networking activities included a two-day annual technical meeting. The main training is the annual CHAPSim users' meeting and training courses in Code_Saturne.

UKTC

With the renewal, the CoSeC support awarded to this consortium has increased from 0.3 to 0.5FTEs per year. This increase, combined with an underspend from previous years, is enabling us to recruit a new member of staff. The CoSeC project lead for UKTC, Prof Dave Emerson and the UKTC PI will agree plans for the new recruit later in the year.

CCP Turbulence

The development will be centred around 3 main areas: (I) testing at scales (32+ GPU) the work done so far for the for decomp2d&FFT and X3div using mainly the NVIDIA tools and targeting NVIDIA GPUs; (II) Porting of decomp2d&FFT to AMD GPU cards and (III) transfer of the development done under X3div into the new framework X3d2 for the modernisation of Xcompact3d. This objective of all this work is to make the framework around Xcompact3d more portable and able to perform on newly available HPC hardware.

Future work will also investigate the expansion of the capabilities of 2decomp&FFT library for example by folly integrating DCT transforms among the available options.

Tomographic Imaging

CCPi

In the next year we aim at launching a GUI for CIL, which will further lower the barrier for users and researchers; we also aim at bringing forward the developments and optimisation of the CIL, CCPi Regularisation toolkit, CILViewer and DVC code.

The main driver of this is the interaction with the users. During phase-III, the team has successfully established collaborations with national facilities, such as ISIS/IMAT, CLF/EPAC, NXCT (UCL and Warwick spokes), international facilities as ESRF, and national or international X-ray centres as QMUL and DTU. Continuing support to such facilities will enhance the impact on the wider XCT community.

Important additions to the CIL will be the GUI, the addition of phase recovery routines, required by ESRF and DTU, the addition of a simple single material beam hardening correction, required by Swansea and industrial partners.

The integration of Digital Volume Correlation as post processing step in Diamond Light Source I12 and DIAD beamline.

Another key activity for the team is the organisation of training events for the CIL and other software that we develop. We expect to run at least 1 training session per year in CIL and for the DVC code. A training session on the cross platform build system CMake is run bi-yearly.

Finally, the collaboration with CCP-SyneRBI will be continued since it has proven to be extremely successful reducing duplication of efforts, and widening the impact that the CIL has on the tomographic community.

CCPSyneRBI

In 2023/24 we will continue working on the recently added new SPECT imaging modality. We also plan to start working with the XNAT database integration and provide sample pipelines for reconstruction of static data via docker integration between XNAT and SIRF. To make installation easier, we will provide a conda installation of SIRF. We will continue our collaboration with CCPi team to employ their Core Imaging Library (CIL) for stochastic optimisation, as well as joint motion and reconstruction estimation. We will also work on handling LPS coordinate system that coincides with the vendor's, including handling of bed position. Finally, we will continue to improve and enhance our SIRF software by introducing error checks for input and more extensive and systematic testing, and we will strive to optimize SIRF performance, e.g. by increased GPU support.

Quantum Computing

CCP-QC

Plans are to Re-establish the aborted condensed matter working package and organise a workshop on QC and condensed matter with NPL and other interested parts of the community. Follow up of Scientific Applications of Quantum Computing: Materials, Chemistry and Biology - September 2023.

4. Resource Planning and Allocations 2022-23 and 2023-24

This section of the report outlines the financial details and resource planning for 2022-23 and looks ahead to 2023-24.

Reset of EPSRC-CoSeC FTE Allocations to Communities

The issue: Following a reduction of the EPSRC-CoSeC budget in April 2018, a mismatch has existed between the number of FTEs awarded to the communities and the number of FTEs STFC can afford. This mismatch is untenable and needs to be addressed. EPSRC have decided to resolve it by decreasing the FTE allocations to the communities. EPSRC have consulted with CoSeC on how best to implement these reductions. CoSeC have considered a number of scenarios, and upon careful analysis of pros and cons, are proposing a 'salami slicing' approach that reduces by 18% the expected allocation to nearly all communities. Details of the proposal are in the next section.

The agreed solution: The current annual budget currently is sufficient for 19 CoSeC FTEs, based on the UKRI STFC costing guide. 1 FTE should be reserved for the CoSeC project Office (a reduction by 1/3 compared to recommendation of the CoSeC review) to fund project management and impact management activities. It should be noted that the funding for the CoSeC leadership (currently Barbara Montanari and Stephen Longshaw) is provided in-kind by STFC. The rest of the allocations

have been revised as summarised in Table 1 in order to fit within the current funding envelope. The weighting factors used are:

- The awarded allocations for the CCPs
- The requested allocations by the HECs at the recent call (given that panel endorsed those requests as 'minimally viable')
- 1 (i.e. not cut) for allocations below 1FTE/y (CCP-QC, UK Turbulence and HEC WSI)
- The cross-cutting Software Outlook activity had already been paused due to the budget shortage

The option offered by EPSRC to hold back resource to create a pot of FTEs to deploy based on a programme-level view has been discarded at this stage. Analysis indicates that inflicting an even bigger reduction on the allocations to the communities would be counterproductive at this juncture.

	Original Allocation (FTEs)	**Revised Allocation (FTEs)**	**Reduction**
Project Office	1.5	1.0	33%
MCC	2.5	2.1	18%
UKCP	1.0	0.8	18%
CCP9	3.0	2.5	18%
CCPNC	1.4	1.1	18%
CCPi	1.5	1.2	18%
CCP SyneRBI	1.8	1.5	18%
CCPBioSim	2.0	1.6	18%
HECBioSim	1.2	1.0	18%
CCP-WSI+	2.0	1.5	18%
HEC-WSI	0.5	0.5	0%
CCP Turbulence	1.8	1.5	18%
UK Turbulence	0.5	0.5	0%
CCP NTH	1.0	0.8	18%
UK-COMES	1.0	0.8	18%
CCP-QC	0.6	0.6	0%
Software Outlook	1.5	0	100%
TOTAL	**24.8**	**19.0**	

TABLE 1: REVISED FTE ALLOCATION BY COMMUNITY FOR FINANCIAL YEAR 2023-24.

Finance information redacted.

5. Metrics 2022-23

This section of the report includes the CoSeC metrics for 2022-23.
The metrics currently used for this programme are defined as:

- Number of citations in peer-reviewed journals of a publication about software supported by CoSeC funded staff. Please note that not all software packages we support have a citeable publication.
- Number of training days delivered by CoSeC funded staff. This metric measures outputs, ie how many people were trained and over how many days.

- Number of publications in peer-reviewed journals authored, or co-authored, by CoSeC funded staff.
- Number of scientific/technical presentations at external events delivered by CoSeC funded staff.

The metrics are per financial year, with the exception of the citations metric, which is for calendar year (for ease of data collection). In the metrics graphs below, the blue line refers to the total number while the orange line refers to the number per scientific/technical staff member. This is useful because metrics are included for any person irrespective of whether they are partially or fully funded by CoSeC. For information, a graph of the scientific/technical staff headcount has also been included.

Overall, the metrics reflect a healthy programme delivering significant impact, especially in terms of code citations (~3,000 in the reporting year) and training days (~2,000 in the reporting year).

The trend in the metrics reflects the evolution of the programme brought about by the changes in communities supported at every renewal call. When considerable changes of the CoSeC communities occur, the metrics tend to decrease, and then recover as the new communities begin to grow their activities through the CoSeC support. For example, the CCP renewal in 2019/20 saw the cessation of the CoSeC support for CCP5, which used to deliver a large number of training days and presentations via CoSeC, as well as contribute hundreds of code citations. The code citation figure now is dominated by UKCP, and CASTEP in particular, which is expanding its user base very rapidly thanks to the introduction of the a world-wide cost-free source-code academic license.

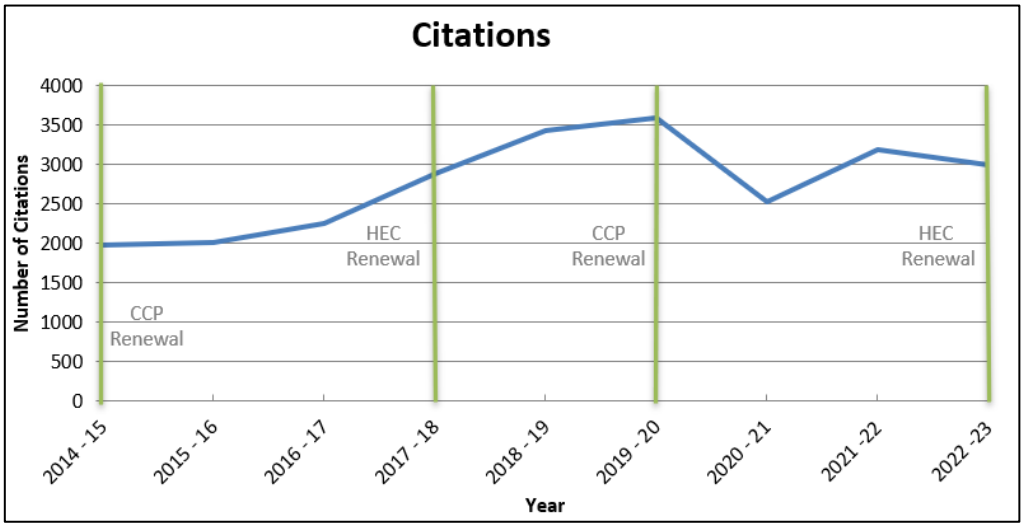
It should be noted that the activities for UKTC were paused for the duration of the reporting year due to staff unavailability. There are mitigating circumstances also for the training days and presentations for UKCP, due to a hiatus in the funding for the consortium itself during this reporting year, compounded by prolonged CoSeC staff illness. The illness of the same person impacted also the delivery for CCP-QC. We expect the staff shortage affecting a few projects to ease in the new reporting year. New staff has been hired and a number of recruitments are in progress.

Metrics breakdown by area

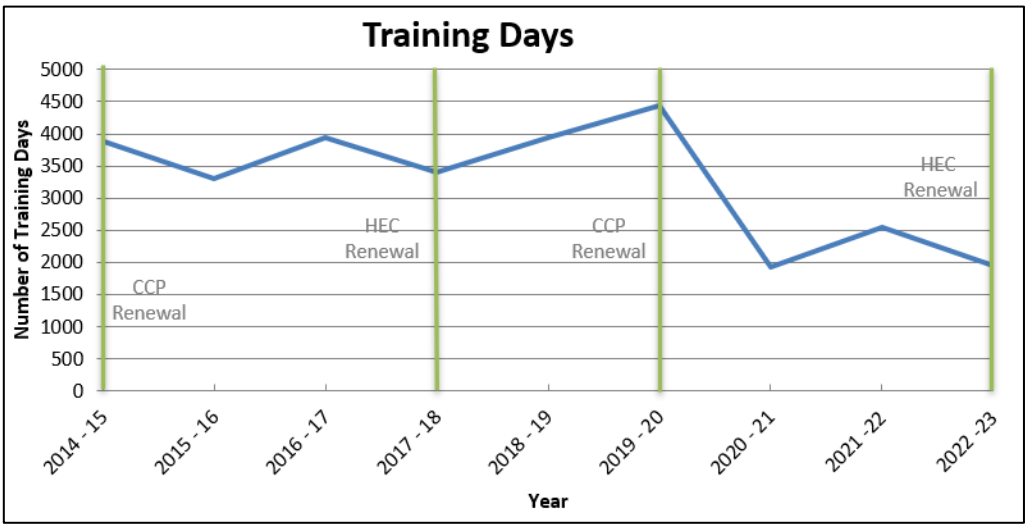
	FTEs Used	Publications	Presentations	Training Days	Citations
Materials Science					
CCP9	2.87	4	5	700	265
CCP-NC	1.24	2	1	208	57
UKCP (including CASTEP)	0.23	1	0	0	1755
MCC (including ChemShell, CRYSTAL)	2.12	11	5	490	692
Biological Science					
CCPBioSim	1.72	0	1	240	17
HECBioSim	0.80	0	3	0	0
Computational Engineering					
UKCOMES	0.40	0	5	30	18
CCP-WSI+	1.90	2	5	0	67
CCP NTH	1.03	2	4	101	2
UKCTRF	0.24	1	2	0	1
UKTC	0.00	0	0	0	0
CCP Turbulence	1.23	0	2	60	0
Tomographic Imaging					

CCPi	1.17	0	3	41	0
CCP SyneRBI	1.78	0	1	25	7
Atomic and Molecular Physics					
UK-AMOR	0.13	1	0	44	118
Quantum Computing					
CCP-QC	0.61	0	0	0	0
Totals	**18.27**	**24**	**37**	**1939**	**2999**

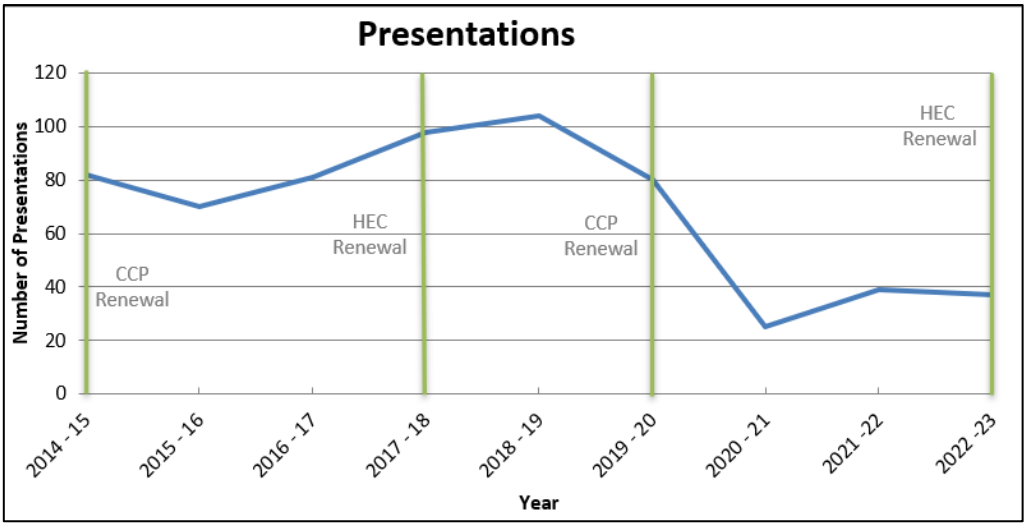
TABLE 4: METRICS BREAKDOWN FOR 2022-23 BY SCIENTIFIC THEME.



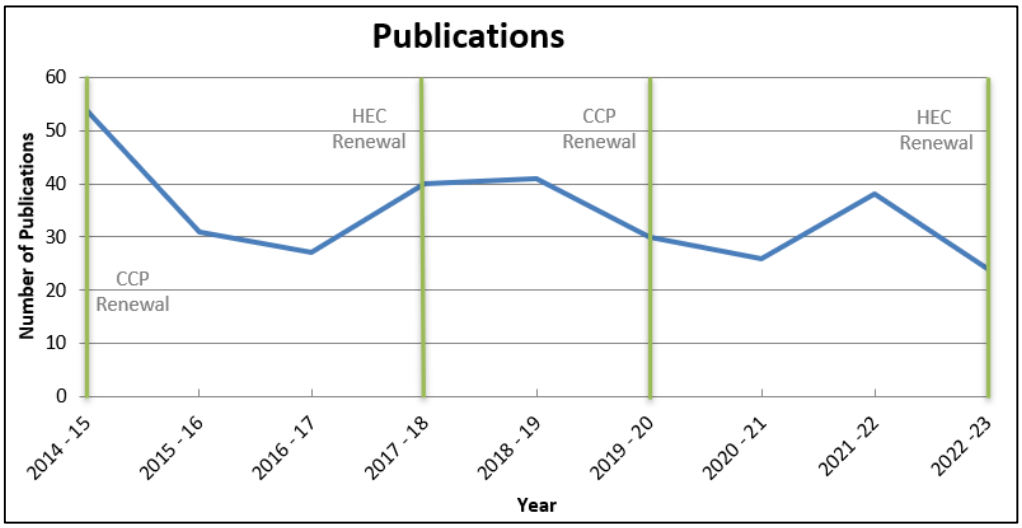
GRAPH 1: COSEC CITATIONS



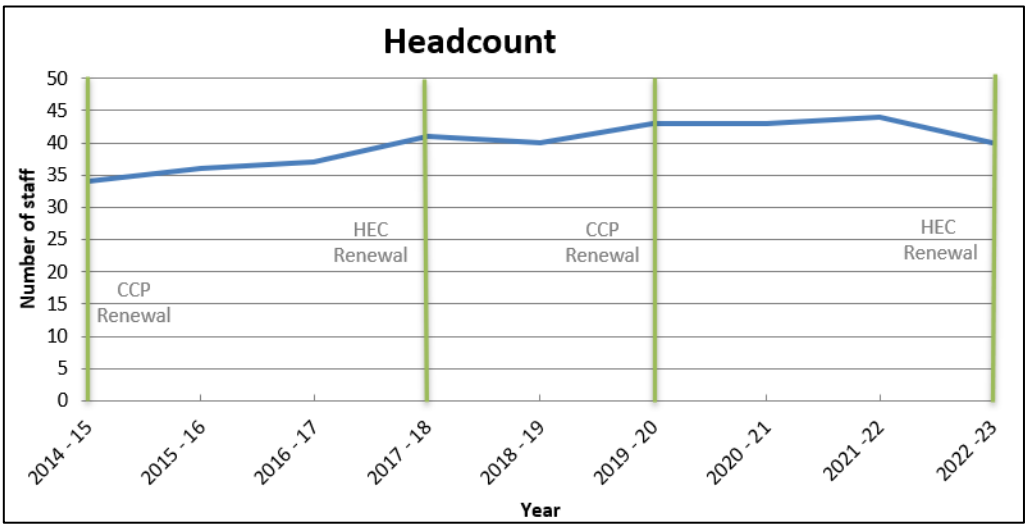
GRAPH 2: COSEC TRAINING DAYS



GRAPH 3: COSEC PRESENTATIONS



GRAPH 4: COSEC PUBLICATIONS



GRAPH 5: COSEC STAFF HEADCOUNT

Community Size

CCP/HEC (Main supported code)	Start Date	Allocation FTEs per year	Community Size April 2021	Community Size April 2023	Method of collection
CCP5 (DL_POLY etc.)	1980	0.00	1050	1484	Active subscriptions to CCP5 mailing list
CCP9 (Questaal)	1981	3.00	450	315 ***	Active subscriptions to the CCP9 mailing list
CCP-NC (MagresView)	2011	1.40	60	133	Active subscriptions to the CCP-NC mailing list
CCPi (CCPi CIL)	2012	1.50	380	437	Two separate mailing lists and one Discord channel
CCP SyneRBI (SIRF)	2015	1.80	80	263	Four separate mailing lists
CCPBioSim (FESetup)	2011	1.95	402 (with HECBioSim)	650 (with HECBioSim)	Mailing lists and HPC Users
CCP-QC	2019	0.60	New Community	70	Active subscriptions to CCPQC mailing list
CCP-WSI+	2019	2.00	169	199	Active subscriptions to CCP-WSI mailing list
CCP Turbulence	2019	1.75	New Community	175	UK Turbulence Consortia distribution list
CCP NTH	2019	1.00	New Community	60	Active subscriptions to CCPNTH mailing list
MCC (CRYSTAL, Chemshell)	1994	2.00	464		
UKCP (CASTEP)	1990	1.00	150	218	HPC Users on ARCHER 2 (plus 1527 academic CASTEP licenses)
UKCOMES (DL_MESO)	2013	0.60	150	250	DL_MESO academic licenses
HECBioSim (Longbow)	2013	0.80	402 (with CCP BioSim)	650 (with CCPBioSim)	Mailing lists and HPC Users
UKTC (Code_Saturne)	2018	0.40	47 (with UKCTRF)	175 (with UKCTRF)	UK Turbulence Consortia distribution list
UKCTRF (SENGA+)	2019	0.50	47 (with UKTC)	175 (with UKTC)	UK Turbulence Consortia distribution list

TABLE 5: COMMUNITY SIZE BY CCP/HEC.

*** Drop in numbers due to a mailing list clean up.

Financial Year 2022-2023 Annual Report

(*Covering the period 1 April 2022 – 31 March 2023*)

APPENDICES

Appendix 1 - Individual CCP/HEC Reports 2022-23

This appendix contains the full, individual summary reports for 2022-23 for the CoSeC supported CCPs and HECs.

Materials Science

CCP9

Wannier90: One of the major tasks within the new CCP9 is the Wannier90 library project, with the CoSeC team, consisting of Jerome Jackson, Barry Searle, Martin Plummer, and Leon Petit, working in close collaboration with the code developers, Arash Mostofi (Imperial College London) and Jonathan Yates (University of Oxford). The goal of this project is to create a parallelized and thread safe library version of the Wannier90, a code that is already interfaced to many community codes and is used to derive advanced materials properties. Interfacing to Wannier90 in library mode will make it more accessible to a larger part of the community, and scientists will eventually be able to access the library through the CECAM electronic structure library (ESL).

Phase 1 (restructuring of argument list), phase 2 (introduction of types) and phase 3 (error handling) are done. This has resulted in a substantially modernized version of the code having improved workflow, readability, and functionality, and this major milestone in has been committed to the public repository. The final phase (phase 4) of the "librification" is done, and we are currently in pre-release testing mode, which will result in a parallel version of the library tested as standalone and on a major plane wave code and also via a new python interface. The librification work was presented at the W90 developers meeting at ICTP by Jerome. Arash presented the project in a presentation at the Psi-k conference in Lausanne. The aim is to present the final product at the W90 developers meeting that is being organized at Daresbury laboratory in May 2023.

The CCP9 Conference and Community meeting was organized at the Crowne Plaza, Manchester, 7-9 September 2022. A number of both invited and contributed talks, panel discussions on the future directions of CCP9, and a poster session made for a very successful event. Jerome and Barry presented the ongoing CoSeC work on the QUESTAAL code and the Wannier90 library respectively. The new CCP9 website (https://ccp9.ac.uk/) was introduced following suggestions from participants at the CCP9 meeting, new content was added over the following months.

After extensive code testing, CRYSTAL23 has now been released. The main additions from the CCP9 side are the hybrid parallelism. Other new features include spin-orbit coupling and g-orbital basis functions. The code and its areas of applications are described in a paper published in a special issue of *J. Chem. Theory Comput.* 2022, https://doi.org/10.1021/acs.jctc.2c00958, with Barry as a co-author.

Manuel dos Santos took part in the ONETEP retreat at Rutherford Laboratory 20-22 September, discussing with the developers the CoSeC work programme on the code. The calculation of the stress-tensor and the optimization of the unit-cell parameters has been implemented and the ability to read pseudopotentials in the commonly used UPF file format is in progress.

The CECAM/Psi-k/CCP9 flagship "4th Daresbury Questaal School" took place at DL. The three-day event had ~20 physically present participants and ~30 via zoom. Jerome gave a tutorial on the QUESTAAL code.

New collaborations in Materials Science: Jerome and Leon visited Didier Sebilleau at Rennes University in the framework of a collaboration to calculate dielectric functions. A publication (Phys. Rev. B **106**, 094402, 2022) has resulted from the TERASWITCH collaboration between Jerome and Sheffield. A

collaboration with Oxford on exchange interactions in 2D Fe5GeTe2 is ongoing. The result of an on-going collaboration between Jerome and colleagues from Hungary on incommensurate magnetic ordering has also been published (J. Phys.: Condens. Matter **34**, 475801). Manuel is continuing his collaboration with Juelich on magnetism in 2D materials, which has resulted in a publication (J. Phys.: Condens. Matter, 34, 454001, 2022).

CCPNC

The CCP-NC has focussed on re-building community outreach and engagement activities as well as engaging directly with feedback from the community. This builds on the communication strategy developed in the previous year.

We have launched CCP-NC Online Meetings: a quarterly online discussion meeting series covering topics relevant to computational solid-state NMR. We have had three meetings to date, with further meetings planned every 3-4 months. The first meetings covered an introduction to the CCP-NC, an overview of the state of the art in computational solid-state NMR, dispersion corrections to density functional theory and crystal structure prediction. The engagement has led to a large increase in the number of subscribers to our newsletter and increased traffic to our website.

In addition, we have launched a travel fund for early career researchers as well as an international engagement fellowship scheme to help promote interactions following the COVID19-related restrictions. CoSeC staff have been involved in the communication of these schemes as well as processing the applications.

Through our refreshed interaction with users, we have identified a number of issues around usability, missing features and documentation in our software and training materials. We have made significant progress in addressing these issues, including a new documentation website for Soprano, and documentation and tutorials on dispersion corrections and transition state searches in CASTEP. In addition, we have made significant progress on a new command-line interface for Soprano that adds a layer of useability to the code, while maintaining the flexibility required by more advanced users. In consultation with a small group of beta-testers, we have also made progress on MagresView2: adding new features and improving the user experience.

Finally, we have written a new software package to tackle disorder in molecular crystals – an original grant objective. This project also functions as part of the CCP-NC's software renewal service as it reproduces some of the functionality in a no-longer maintained code. In addition, we are collaborating closely with the Cambridge Crystallographic Data Centre on this project.

UKCP

The annual CASTEP core developers coding workshop (a.k.a. "Codefest") was held in person in April 2022 and March 2023. This brings the core developers together to focus on collaborative coding projects, agree strategy, roadmap future developments, and reflect and build on software best practices used.

Since 1st April 2022, an additional 411 groups have obtained a free of charge academic CASTEP licence. September 2022 saw the delayed release of academic CASTEP 22.1.1 to coincide with the in-person teaching workshop for CASTEP users. Preparation for the academic release of CASTEP 23.1 in May 2023 was done. This included extensive tests of refinements to the existing GNU make build system and a new cmake build system developed by Jacob Wilkins (STFC, SCD) and Keith Refson (STFC, ISIS). These tests aim to provide a robust and relatively straightforward way for users to take the source code as distributed to a usable software tool. The cmake system will benefit users in the community by greatly simplifying deployment of CASTEP on Microsoft Windows computers.

Effort for UKCP during this period has unfortunately been disrupted due to staff illness. As a result, code development projects for a CASTEP-YAMBO interface and an implementation van der Waals-DFT in CASTEP have been put on hold to be resumed when staff effort allows.

MCC

Benchmarking: Benchmarking efforts in this period focussed on ensuring that DL_POLY and LAMMPS produced the same scientific results in order to reliability assess their scalability. Planned tasks for this period comparing simulations employing only non-bonded interactions in DL_POLY and LAMMPS, and bonded interactions in the same codes, have been completed and will be reported at a future MCC meeting. Work to choose codes and test cases for periodic DFT benchmarking is ongoing.

CRYSTAL and ExCALIBUR: CRYSTAL23 was released in Dec 2022. The new release was made available to MCC users on Archer2 in Jan 2023.

One of the main factors in the performance of CRYSTAL is the distributed matrix diagonaliser. Currently SCALAPACK is employed, but due in part to the various exascale efforts worldwide several alternatives are available. The feasibility of using ELPA on ARCHER2 has been examined, and these investigations continue as part of MCC support for the ExCALIBUR project, to form a comparison with GPUs.

ChemShell: After rigorous testing both the legacy Tcl-ChemShell and redeveloped Py-ChemShell packages have been made available as centrally installed modules on ARCHER2. As an open source package the Py-ChemShell module is available to all ARCHER2 users. Py-ChemShell has been interfaced to the MolSSI basis set library via its standardised API, offering a simple and flexible way to select basis sets in QM calculations. The embedded cluster model for covalent materials has been benchmarked using the hybrid MPI/OpenMP QM code LSDalton, in comparison to NWChem. Py-ChemShell continues to be maintained on both ARCHER2 and Tier 2 systems such as UCL's YOUNG facility, together with the legacy Tcl-ChemShell package.

DL_POLY: As an open source package DL_POLY module is available to all users, including those of ARCHER2. Support has been provided to ARCHER2 and Tier2 users at QMUL. Work to advance on-the-fly capabilities has began in December 2022, funded by EPSRC Software for Communities call. General "on-the-fly" correlator module has been written and tested against VAF, already existing but not "on-the-fly". Comparison and testing have been completed, the version is tagged and the feature is being documented prior to release.

DL_FIELD: The COMPASS force field for general organic molecules in the condensed phase has been implemented within DL_FIELD, containing all data that are in the public domain. Work to improve the automation of organic-inorganic non-bonded interactions through interconversion of potential functional forms is in progress and expected to complete as planned. Specifically, DL_FIELD can automate refitting of Morse potential to LJ12-6 form for vdw mixing. These functionalities are made available through the latest release (4.9). In addition, programming infrastructure has been developed for DL_FIELD to recognise third-party force field (FF) file format. This enable DL_FIELD to setup FF models derived from third-party FF database. For instance, FF derived from LigParGen can now be readily transcribed into DL_POLY format.

Biological Science

CCPBioSim

The CodeEntropy project has been successfully completed which saw work to bring together the existing codes for calculating the entropy of proteins and solvent. The code was also rewritten to take advantage of MDAnalysis and its trajectory parsing functionality. CodeEntropy has been released

(https://github.com/ccpbiosim/codeentropy) and the documentation is available (https://codeentropy.readthedocs.io). There was a hackathon in January with 10 participants which directed the writing of a proposal for 12 months work to improve the functionality and user friendliness of the code. We are planning to include CodeEntropy in the next CCPBioSim Training Week.

The CCP website has been rebuilt based on the Joomla 4 platform with a new look and feel, new logo and a more focused set of page content to respond to the advisory board recommendations. The slimmd database has been ported over to the new website and the interface simplified and a new categorised layout and data model developed.

The training platform has been completely rebuilt using the latest stable operating system (Ubuntu 22.04) for the VMs and switched onto k3s kubernetes which is a lighter fork of mainline kubernetes. The websites and training platform have now been brought under the scope of the same cluster where the metrics and analytics could be expanded to assess where community user traffic is flowing. The training course containers have been updated to the latest versions of operating systems, jupyterhub and all software packages updated, these have then been tested and issues arising from updates have been recorded and reported to authors. The containers have been migrated off of dockerhub due to sun-setting of free tier access, and migrated to STFC hosted harbour which has also improved container pull times. The metrics have also been expanded for training notebooks, so we can now get access to a very advanced set of telemetrics about how our training resources are used.

Work has begun on the ensemble docking workflow project. This project involves a series of Jupyter notebooks which contain a workflow for docking ligands (small molecules) to multiple protein structures to allow for the investigation of the effect of conformational changes or mutations on the ligand binding. The notebooks and relevant software will be packaged into a virtual machine to enable them to be shared easily.

The finite temperature string method project is making progress. It has been decided that it will be a standalone utility rather than a feature of other codes. The example scripts have been reviewed and comments added. Some code refactoring is still required, but it is on track.

The FFEA project has progressed to the stage where the majority of the numerics have been integrated into the Code_Saturne package, the work on this project has now been moved to an eCSE grant where the remaining integration work will continue alongside pilot scaling studies.

The CCPBioSim Training Week was run as a hybrid event this year. See the training section for more information.

The Industry Talk series continued to be popular with our community. The talks since 1 April 2022 have included speakers from Vertex (59 participants), Merck (53 participants), Astex (62 participants), NPL (20 particpants) and OpenBioSim (66 participants).

HECBioSim

In the current reporting period to date considerable work has been done supporting new users getting set up and running on ARCHER2, JADE2 and Bede. In this reporting period the HEC has changed the way that it offers applications for HPC to a single panel each 6 months at which applications are invited for access to all HPC facilities. This has required significant updates to the online application structure, the guidance for PIs and also in the way RAPs are supported. The CoSeC element supporting RAPs now focusses on the technical assessment of scientific cases against the resource requests and studies are now automatically placed upon the optimal HPC resource based on benchmarking and specialist expertise.

Critical operating system and performance updates applied by the Bede system administrators required a complete rebuild of all software packages made available under HECBioSim, this required significant effort to rebuild and test each package for correctness and performance against benchmarks to ascertain that historical numerical and communications issues on the platform had not remerged.

The project to test compile our supported software on UK Tier2 Wilkes3 (Cambridge) and Sulis (Warwick) and then benchmark the machines with the HECBioSim benchmark suite has been completed. The results have been published on our benchmarking webpages on the HECBioSim website and the data added to our resource calculator and will be available in the near future. This work will form the basis for running a call for access to these two machines and will allow us to show the community how to get high performance from the new Nvidia Ampere architecture.

The project to connect the benchmarking suite data outputs to the online calculator in an automated way has been completed. The work involved creating a set of data extraction scripts to capture the raw benchmark outputs and feed it into a set of data models to extract the underlying scaling patterns. This then can be used as the underlying data model behind the HEC calculator. This work will simplify future work on adding new codes and a much simpler route to monitor new release versions of existing software and allowing us to update the calculator more frequently.

Work on Longbow 2.0 has continued with additions to the code base supporting more advanced ways of connecting with HPC clusters. However, further work has been paused whilst we review the consequences of recent implementation of 2 factor authentication on SSH by a number of computing centres and what this means for Longbow operation. This security measure has been applied to one of the key components that Longbow uses to communicate with HPC machines and since it is a security feature should not be circumvented, we are currently considering a slightly different operating model, or retire the code entirely.

Work has also focused on supporting consortium users with technical issues arising with constantly changing system environments, and in particular issues with building newer versions of software that are problematic. These issues relate to openmm and AMBER 22 on JADE2, the issues have been identified within the system build environments, fixes are being prepared for deployment in the near future.

Work to scope two future projects has completed, one to expand the benchmarking suite to add openmm and code_saturne and the other to scope a project around AI driven MD. The findings of the scoping exercise have informed plans within the new HEC cycle if the renewal is successful.

Computational Engineering

UK-COMES

Preparations for a new release of DL_MESO are in progress, which is expected in Q2 2023. Prior to this release, improved input file reading and restart file writing have been added to the LBE code to ensure it can run efficiently on larger numbers of processor cores. A interface to the PLUMED library has been added to the DPD code to provide enhanced sampling and analyses, as well as enable free-energy methods to explore phase transitions and other transformative phenomena. Trajectory file writing in netCDF has also been added to the DPD code, automating the process of including metadata with simulation trajectories to make them FAIR (findable, accessible, interoperable and reusable) when added to data repositories.

A few high-level C++ elements have been designed and are being implemented to automatically integrate contributions to MPLB/HiLeMMS. A PhD student from the Cardiff University, Mr Baoming Guo, has been at DL for a one-year visit. He was trained to use the HiLeMMS system for his research and has been developing its free surface flow capability.

CCP-WSI+

HEC-WSI: Due to a delay in the HEC-WSI project starting because of some technical issues with the original proposal, it was approved by EPSRC around the start of March 2023. To ensure the HEC was able to start on time, a new website has been created at www.hec-wsi.ac.uk and populated with a skeleton framework for requesting ARCHER2 time. A more detailed CoSeC update will be provided during the next reporting period.

CCP-WSI+: During this reporting period each work package of the CoSeC support for the community has progressed in a number of ways, this is detailed below. A new Software Strategy has also been created for the community in consultation with the University of Plymouth, which will be reviewed, refined and actioned over the coming reporting period. This aims to formalise all of the ongoing threads of activity wrapped up in WP1 and WP2 and present a picture of how it all fits against a key problem type for the WSI community, the floating offshore wind turbine.

WP1: Work during this reporting period has continued to focus on creating software capability for the types of WSI modelling problems important to the CCP-WSI+ community. Ongoing developments to the open-source Parallel Partitioned Multi-physics Simulation Framework (ParaSiF - https://github.com/ParaSiF/ParaSiF). This work has been looking at implementation of the structural and fluid solvers from ParaSiF into their latest respective framework releases (FEniCSx and ESI OpenFOAM). It has also considered modification of the interFSIFoam and pimpleFSIFoam fluid solvers from ParaSiF to incorporate new generic coupling algorithm support from the MUI library, utilising a new lightweight integration of MUI into ESI OpenFOAM.

Developments to the Multiscale Universal Interface (MUI) code coupling library have happened on the back of developments to ParaSiF, these have resulted in a new generic coupling algorithm capability and a self-contained custom linear algebra capability with the expectation of a major release early on the next reporting period. This new capability presents a generic capability applicable to a variety of problems found in the WSI community.

The CCP-WSI+ blind test series considering the interaction of a thin flexible membrane is also being used as a scientific driver to develop new capability within the structural solver of ParaSiF, with a submission to a dedicated session ISOPE conference underway.

WP2: Work during this period has focussed on dynamic load balancing for the latest version of ESI OpenFOAM, developing stand-alone fast, low overhead domain decomposition and dynamic load balancing in the form of parmetisDecomp. This is released via the ccp-wsi-new GitHub repository (https://github.com/CCP-WSI/ccp-wsi-new/tree/main).

During this period, profiling interFoam using 1024 MPI tasks has also been completed, using ARCHER2, this led to the ARCHER2 support team identifying a bug in the perftools-base/21.02.0 modules and resulted in a fix (Q1897343). The MUI library has also been integrated into the new CCP-WSI repo as third party library without changing the source code of the latest versions of ESI OpenFOAM. This has been tested on ARCHER2, including installation and development of SLURM scripts needed for running partitioned coupled jobs. This WP has also explored parallel fluid-fluid and fluid-structure coupling using an alternative coupling library, preCICE, and contributed to the CCP-WSI+ blind test series with University of Plymouth.

WP3: The main CoSeC lead for this WP has been on secondment to UKRI for the majority of this reporting period, however there are still highlights from this work package to report. The catalogue framework for Projects and Test Cases had been released. The cataloguing framework encourages and enables engagement with the CCP's community. Any member of the CCP-WSI organisation on GitHub, (controlled by the Working Group) can log on and add new Test Cases and related projects to the catalogues. Furthermore, the catalogues are linked so if a project is related to a Test Case or another project this can be specified in the meta data. This results in a well-connected framework which enables users to easily learn what work is being done within the community. The potential the cataloguing framework has, not just for the WSI domain, but also at a higher level (e.g. CoSeC wide) is a very exciting prospect.

Another highlight for this WP has been the development and release of the new HEC-WSI website as reported above, which is a time critical exercise and successfully delivered with online forms made live in time for the launch. Finally, news from the community continues to be disseminated from the website and support for all events (eg registrations) given.

CCP-NTH

The main code development task of CCP-NTH is the code development of the community code, CHAPSim, to increase its numerical accuracy up to 6th order accuracy and to increase its parallel capability. High order accuracy for spatial discretisation enables CHAPSim to capture subtle characteristics from turbulence and heat transfer with limited numerical dissipation. The multi-dimensional parallelisation makes CHAPSim use of the latest advanced distributed-memory HPC systems (i.e. ARCHER2).

During this reporting period, new functions have been implemented to CHAPSim2 to support research in the CCP-NTH community. (1) A pre-/post-processing for staggered grid applied to the Poisson equation has been implemented. Sine/Cosine transformation has also been implemented to the code for FFT to handle Dirichlet and Neumann boundary conditions. The Sine/Cosine transformation has been implemented into the open-source library 2decomp&FFT which is maintained by the CCP-Turbulence, and this will benefit a broader community than CCP-NTH's. (2) Paraview compatible format 'xml' for data output including raw data and space/time averaged data has been added to CHAPSim2, which benefits users for a consistent data post-processing. (3) The parallel performance of CHAPSim2 has been carried out on ARCHER2. The software has been successfully tested using up to 256 nodes (32,768 MPI tasks) for a test case with a mesh having more than 1 billion cells. (4) The cylindrical coordinates to CHAPSim2 with high order compact schemes and 2decomp&fft lib for pipe or annular flow simulation is carrying on. (5) CCP-NTH supports the code development of immersed boundary condition (mainly carried out in the University of Sheffield) to CHAPSIm2 to simulate flows over arbitrary objects. CCP-NTH supports the code development of multiphase flow (mainly carried out in STFC via eCSE project) to CHAPSim2 to simulate boiling flow.

There are two milestones during this reporting period: (1) at the 2022 Annual Technical Meeting in June, a pre-release version of CHAPSim2 was introduced to the CCP-NTH community. (2)A full new version of CHAPSim2 for Cartesian coordinate is released in November to CHAPSim2 users and the community.

UKCTRF

SENGA+ is one of the key DNS codes in the UKCTRF for studying fundamental flows with simplified chemistry. Over the last year, the comprehensive NSCBC boundary conditions, which include the transverse and diffusion terms, were implemented in the SENGA+. As the result, the prediction of the flame was improved significantly when it approaches the computational domain boundary.

SENGA 2 is a sister code of SENGA +, which is a dimensional code with detailed chemistry. Implementing the transverse and diffusion terms in the NSCBC boundary condition for SENGA 2 will improve the performance of the code and increase the simulation accuracy close to the boundary.

Derivation of the boundary conditions in 3 directions has been done. The implementation of the boundary conditions is still ongoing. A spherical flame configuration has been set up to test the implementation. No satisfactory results have been obtained yet.

UKTC

Staff availability issues made delivering the 0.3FTE for this consortium not possible this year. The underspend resource will be delivered once a new recruit is in place. A small amount of work was undertaken to scope out how we could integrate particle tracking into Xcompact3d. The consortium has benefited from the software support for other communities that are synergistic with it, such as CCP Turbulence and UK COMES.

CCP Turbulence

A new release of the 2decomp&FFT library has been released which support NVIDIA GPUs offloading as well as a back end for CUDA FFT to perform FFT Fast Fourier Transform on the GPU (https://github.com/xcompact3d/2decomp-fft). The decoupling of 2decomp&FFT from the main branch of the Xcompact3d will help in increasing the impact since the library is used by several codes to perform 2D decomposition. For example the code CaNS is already using the new release of the library linking directly to the newly created repository (https://github.com/CaNS-World/CaNS/tree/main/dependencies).

A full Navier-Stokes solver has been added to the X3div mini-app and ported to GPU (https://github.com/rfj82982/x3div/tree/2d-decomp-fft_external_library) and it is now using the decomp2d&fft library as and external dependency.

Work has also been done on adding particle tracking to the main Xcompact3d solver (MPI only). The developments now include: (I) possibility to give mass, size, and density to the particle, (II) addition of both fluid force and magnetic force to the particle tracking and (III) improvements of the integration method to alleviate the small-time step required by the ODE problem. Development are available in https://github.com/rfj82982/Incompact3d/tree/dev-stfc-particle

In the first part of the year, a python code generator was developed for implicit type high-order finite difference schemes based on the OpenSBLI system. The purpose is to help to use such schemes by manipulating equations in concise tensor form. Parallel IO facilities are developed into the OPS library for writing out arbitrary section of the computational domain onto the disk. This can help greatly reduce the IO time during simulations.

Tomographic Imaging

CCPi

Software development, maintenance and distribution: development of the Core Imaging Library (CIL https://www.ccpi.ac.uk/CIL) with extended support for input of Nikon and Zeiss lab X-ray machines, optimisation of functions and new ISTA algorithm for the iterative reconstruction module, code refactoring, deprecation and removal, merger with CIL-ASTRA repository with relicensing. Development of the interactive 3D viewer (CILViewer) with new readers and refactoring of the main classes.

Collaborations:

- With ISIS/IMAT to provide CIL powered iterative reconstruction. A solution for Least Squares with TV regularisation with PDHG and SPDHG algorithms have been developed

- With European Synchrotron Radiation Facility beamline ID15 to provide a standard CT reconstruction pipeline, with the development of a new ad-hoc reader.
- With Warwick Manufacturing Group for the use of iterative algorithms on large CBCT data, with particular emphasis on algorithms stopping criteria and optimisation.

A joint hackathon with CCP SyneRBI and PET++, took place on 4 to 7 April 2022. The goal of this hackathon was to establish a suitable reconstruction evaluation strategy, including metrics for image quality and algorithm performance (run-time, memory etc.), taking into account parameter selection for algorithms used.

CCPi, together with CCP SyneRBI, supported QUIERO Workshop on Cardiac MRF Simulation & Evaluation, held on 6 July 2022 in Berlin, that provided participants with hands-on experience on simulation of MRF data acquisition and evaluation of T1 and T2 maps in clinical practice and using advanced machine learning approaches.

On March 20th to 23rd the team organised a 2 day hackathon as side event of the Rich Tomography Workshop held at the Isaac Newton Institute in Cambridge. The event aim was to enable new users to use CIL in their own research. 30 participants joined from the UK and Europe.

The CIL developers team participated into the Helsinki Tomography Challenge, an open challenge organised by the Finnish Inverse Problems Society on limited angle CT. The team's algorithm developed in CIL, granted the 3rd place in the competition.

CCPSyneRBI

Our work during the reported period mostly progressed according to the job plan. We continued our software development and engineering efforts, adding content to our website www.ccpsynerbi.ac.uk, maintaining our mailing lists, organising online meetings, training courses and Hackathons.

On 6 July 2022 we released SIRF 3.3, our first release that adds a new modality SPECT (Single Photon Emission CT) to the two modalities, PET and MR, we have been covering in all our previous releases. This is a major step forward for our Synergistic Image Reconstruction Framework, enabling for instance applications in theragnostics, where PET and SPECT are often used for planning and monitoring of treatment.

Our 9th Hackathon, joint with CCPi and PET++, took place on 4 to 7 April 2022. The goal of this hackathon was to establish a suitable reconstruction evaluation strategy, including metrics for image quality and algorithm performance (run-time, memory etc.), taking into account parameter selection for algorithms used. This will lead to an open framework for evaluation of image reconstruction algorithms, as well as at least one journal paper. Together with CCPi, work is now nearing completion on a general implementation of stochastic optimisation algorithms in CIL. This will allow us to provide faster reconstruction algorithms as well as performing research on novel ways to speed-up reconstruction in the case of motion as well as multi-modality data.

Our most recent version 3.4 of SIRF was released on 19 Jan 2023. New features include support for spiral MR acquisition trajectories, writing MR images to DICOM files, support for latest version of Gadgetron, support for Pinhole SPECT (to the best of our knowledge a first for open source software) and extraction of subsets of acquisition data. Many of these features were contributed by SyneRBI members but checked and finalised by CoSeC.

CCP SyneRBI co-sponsored XNAT Workshop in London 31 Oct to 4 Nov 2022, which provided hands-on time with expert XNAT developers for newcomers and experienced stakeholders alike. The workshop and associated hackathon was attended by Edoardo Pasca (and other SyneRBI members)

which resulted in a prototype implementation of the XNAT plug-ins for being able to incorporate raw MR data and run SIRF reconstructions.

We have also started transitioning the SyneRBI website from Drupal to the new WordPress platform.

Atomic and Molecular Physics / Plasma Physics

UK-AMOR

With limited support of 0.2FTE which ended at the end of December (following the start of the new HEC funding round) activities have concentrated on new funding opportunities. MP supported the UK-AMOR HEC renewal bid (led by Professor Hugo van der Hart, QUB who is taking over new activities from Professor Tennyson). He was co-I on an EPSRC responsive grant application (PI Dr ML Law, Aberdeen) to study and predict reactive antihydrogen interactions with molecular hydrogen of great relevance to the CERN ALPHA project (and related projects) for the production, spectral study and future use of antihydrogen atoms. The proposal had very strong referee reports but was sadly ranked beneath the funding cut-off by the December Physics panel. MP is a key worker on an ARCHER2 eCSE proposal to upgrade substantially a new code (PI Dr Dermot Green, QUB, with co-I Dr Charles Patterson, Trinity College Dublin, project workers MP and Alin Elena) studying positron interactions (binding, annihilation, spectra) with organic molecules. The eCSE proposal was successful and the project started in Q4 2022. MP began collaborative work with an Ada Lovelace Centre (ALC) project in SCD studying spectroscopy of muonic atoms, relevant to the STFC ISIS facility (muon-based analysis of materials) and he will be partially funded by that budget in Q4 2022 – Q1 2024. Indeed, an ALC PhD studentship (50% funded by ALC, 50% funded by the University of Warwick) was awarded to this project (in the UoW HetSys CDT) to begin in October 2023 with MP as a research supervisor (joint supervision by SCD, ISIS and UoW).

The UK-AMOR proposal, which planned for expansion of the community and a full CoSeC support programme (similar to previous support for CCPQ) was rejected by the EPSRC panel. The official EPSRC UK-AMOR network ended in late January 2023, however its members will continue to collaborate on AMO projects.

In addition, MP carried out follow-up work to an ongoing ARCHER2 eCSE project which ended in May, on optimization of the UK-AMOR flagship RMT code for laser atom/molecule interactions, achieving substantial performance improvement [and continued supporting separately funded work as a co-I on the EPSRC 'AQuA-DIP' grant to introduce double-ionization capability to RMT]. A paper has been submitted to Frontiers in Physics (as part of an AMO Editor's Challenge Special Topic) on the antihydrogen work (E Kasoar, M Plummer, L van Lydon, MM Law) using material from E Kasoar's Graduate project with MP. CoSeC project management collected registrations for the 'CCPQWindsor 2022: Dynamics of Complex Quantum Systems' conference, 25-28 July 2022 and is collecting registration for the AQuA-DIP conference Quantum Battles in Attoscience to be held at UCL and online, 28-30 June 2023.

Quantum Computing

CCP-QC

Planned activity was around Quantum Computing for Condensed Matter Simulations, with CoSeC support from Dr Dominik Joachim. Unfortunately, due to medical issues, long covid, the workpackage was delayed and measure put in place to anticipate Computational Engineering package that will happen Q4 2022 and Q1 2023.

Planned mini-colloquium on Quantum computing and Condensed Matter Simulations went ahead as planned, during CMD 29 EPS-IOP August 21-26, 2022 Manchester. Event was weill attended run in

hybrid mode, with invited speakers from Google Inc, University of Michigan and Freie University Berlin. 30 attendants were present. The workshop was organised by Francois Jamet, National Physical Laboratory, Martin Kiffner University of Oxfrod, Liviu Chioncel University of Augsburg, Germany, Alin Elena, Daresbury Laboratory STFC.

Working group 4 around QC and Computational Engineering, happened during Q4/22 and Q1/23. Regular meetings between specialists in both fields happened over zoom, culminating with a face to face event in January 2023 at Daresbury Laboratory. A Comprehensive review of literature of interest it is under way by members of the group.

Follow up events are planned beyond.

Appendix 2 - Individual CCP/HEC Work Plans 2023-24

This appendix contains the full, individual work plans for 2023-24 for the CoSeC supported CCPs and HECs. Tasks highlighted yellow indicate a change from the plans submitted in the interim report, November 2022, a task that has been removed, or a new task that has been added.

Project Office

Project Office	Milestone	Target Date
Project Management	Attend CCP and HEC committee meetings as required	Ongoing
	Support CCP and HEC conferences and workshops as required	Ongoing
	Weekly internal STFC meeting to discuss progress with all CoSeC activities	Ongoing
	Monitoring of staff effort and spend on a monthly basis	Ongoing
	Financial forecast and costing for 2023-24	Q2 2023
	Arrange internal project meetings with funded CCPs and HECs – April 2023 – meetings arranged by scientific field	Q2 2023
	Prepare and submit CoSeC annual report – June 2023	Q2 2023
	Arrange and attend the CCP Steering Panel May meeting	Q2 2023
	Attend the CoSeC SLA Steering Committee June meeting	Q2 2023
	Arrange internal project meetings with funded CCPs and HECs – July 2023 – meetings arranged by scientific field	Q3 2023
	Compile and submit ARCHER renewal proposal	Q3 2023
	Arrange internal project meetings with funded CCPs and HECs – October 2023 – meetings arranged by scientific field	Q4 2023
	Prepare and submit interim CoSeC SLA report – November 2023	Q4 2023
	Arrange and attend the CCP Steering Panel December meeting	Q4 2023
	Attend the CoSeC SLA Steering Committee December meeting	Q4 2023
	Arrange internal project meetings with funded CCPs and HECs – January 2024 – meetings arranged by scientific field	Q1 2024
Impact	Write and publish news articles and case studies on the CoSeC website	Ongoing
	Define CoSeC impact role within SCD group structure	Q1 2023

	Administrate CoSeC Impact Award	Q2 2023 – Q1 2024
	Write and publish CoSeC Impact Award 2023 case studies	Q3 2023 – Q4 2023
	Launch the CoSeC Impact Award 2024	Q1 2024
	Facilitate and oversee creation of 6-12 impact studies	Q4 2023
	Create and publish CoSeC impact report based on impact studies	Q4 2023
Technical	Scope new working group areas and facilitate their start and goals	Ongoing
	Scope and produce tangible outputs from working groups where appropriate (i.e. white-papers, group publications etc.)	Ongoing
	Scope and create internal CoSeC skill-sharing exercises.	Q2 2023
	Scope new CoSeC open journal special edition as outlet for annual conference	Q2 2023
	Organise and run third CoSeC Conference	Q3 2023 – Q4 2023
	Chair and maintain CoSeC Conference committee	Q3 2023 – Q4 2023
Strategy / People / Relations	Represent CoSeC on the National and International arena	Ongoing
	Oversee the resourcing and delivery of the CoSeC workplan	Ongoing
	Oversee the CoSeC staff professional and career development	Ongoing

Materials Science

CCP9	Milestone	Target Date
	W90 developer's meeting	Q2 2023
	Publish paper on magnons in Mn5Ge3	Q2 2023
	Publish paper on spin-phonon coupling in magnetic nanostructures	Q2 2023
	ONETEP: spin-orbit implementation	Q3 2023
	ONETEP: GPU feasibility study	Q3 2023
	Workshop: First-principles Green function formalisms	Q3 2023
	Publish work on magnetic properties of Mn2Au	Q3 2023

	QUESTAAL 7.16 release	Q3 2023
	QUESTAAL: BSE spin susceptibilities	Q4 2023
	Publish black Phosphorous paper	Q4 2023
	CCP9 Community meeting and Conference	Q1 2024
	Enhanced CCP9 website (repo/archive/working groups)	Q1 2024
	SPR-KKR Study of Ru based Heusler alloys	Q1 2024

CCPNC	Milestone	Target Date
	Organise quarterly CCP-NC Online Meeting Series	Ongoing
	Maintenance of the CASTEP-ASE interface: complete refactor of the input/output modules	Q2 2023
	Finalise and document the Soprano command line interface for common NMR workflows	Q2 2023
	Full release of SODORG Python code	Q3 2023
	Replace existing API for the CCP-NC database	Q4 2023
	Finalise and document the Soprano command line interface for common NMR workflows	Q4 2023
	Rebuild CCP-NC database software stack, replacing AngularJS	Q2 2024
	~~Achieve functional equivalency between MagresView 1.0 and 2.0~~	~~Q1 2024~~
	Major Soprano release: restructure and document core features with usability as priority.	Q1 2024

UKCP	Milestone	Target Date
	Management of Academic CASTEP user licensing and source code distribution.	Ongoing
	Management of CASTEP code repository and continuous integration system.	Ongoing
	Co-organization and teaching for CASTEP workshop in Oxford.	Q3 2023
	Deployment of Academic CASTEP licence query service for HPC administrators.	Q4 2023
	Organisation of 2024 CASTEP "codefest" core developer workshop.	Q1 2024
	Release management of Academic CASTEP v24.	Q1 2024

	Report on error quantification of DFT pseudopotential in hybrid DFT calculations.	Q1 2024
	CASTEP-YAMBO interface	On hold
	CASTEP implementation of van der Waals DFT	On hold

MCC	Milestone	Target Date
	Coordination of MCC CoSeC support and recruitment of additional staff to provide CoSeC effort	Q1 2024
Ab initio DFT	Recompile, test and maintain CRYSTAL23 on ARCHER2 following the programming environment upgrade	Q3 2023
Classical and ML forcefields	Benchmarking of ML interatomic potentials for structure and dynamics of MOFs, comparing HDNNP, MACE and NEP vs classical forcefields	Q1 2024
	Hold an MCC DL_POLY user group workshop, and plan a hands-on training workshop for the following year	Q4 2023
	Add capability to read CHARMM RTF and PRM files into DL_FIELD, to enable access to third party FF webservers (LigParGen, MATCH)	Q2 2023
	Implement all-atom TraPPE forcefield in DL_FIELD for studies of phase equilibria of some industrial chemicals	Q1 2024
	Implement Hill-Sauer zeolite FF in DL_FIELD, including compatibility with similar FFs already implemented	Q4 2023
	Release DL_FIELD version 4.10. Testing, manual and tutorial updates	Q4 2023
Multiscale methods	Recompile, resolve issues and maintain ChemShell/NWChem/GULP on ARCHER2 following the programming environment upgrade	Q2 2023
	Report on LSDalton and NWChem benchmarks for zeolite systems on ARCHER2 (including comparison of standalone execution and via ChemShell).	Q3 2023
	Extend subtractive QM/MM functionality in Py-ChemShell to periodic MM environments via GULP, and test on materials systems	Q4 2023
	Add automated support for zeolite QM/MM calculations in Py-ChemShell via DL_POLY and DL_FIELD, and update the corresponding online tutorial	Q1 2024
	Integration and validation of ML optimisation methods into DL-FIND release	Q1 2024

Biological Science

CCPBioSim	Milestone	Target Date
Manchester Multiscale Conference	Run the 5th Manchester Multiscale Conference. There will be 8 invited speakers and about 16 contributed talks plus posters	Q2 2023
Enhanced Sampling Project	Collaborate with Edina Rosta (UCL) to implement her finite temperature string method into Plumed.	Q3 2023
Online Training	Add modules to the online training (ProDy, BigDFT, maybe oxDNA or others as needed for training events)	Q4 2023
New Short Software Project	Details to be determined	Q1 2024

HECBioSim	Milestone	Target Date
	Support the consortium users of HPC with ARCHER2, JADE2 and Bede with performance issues, software issues, running issues, questions on how much resource etc.	Ongoing
	Maintain the HECBioSim benchmarks with regular tests on new software releases across Tier 1 and Tier 2 HPC	Ongoing
	Maintain HECBioSim webserver and website	Ongoing
	Maintain the Longbow software package	Ongoing
	Support HECB post-doc with AI for MD project development	Ongoing
	Migrate website to Joomla 4 (Current Joomla 3 end of life mid 2023)	Q2 2023
	Develop first new training course for HPC	Q3 2023
	Create benchmarks for OpenMM that match the HEC benchmark suite.	Q4 2023
	Develop second new training course for HPC	Q1 2024
	Expand benchmarking suite and HEC calculator to include multi-GPU information and more physics within each package.	Q1 2024

Computational Engineering

UK-COMES	Milestone	Target Date
HiLeMMS	Further integration of AMReX code for adaptive mesh refinement capability	Q1-2024
DL_MESO	Interfaces in DPD and LBE codes to enable coupled simulations	Q1 2024

CCP-WSI+	Milestone	Target Date
	Investigate the scalability of linear solvers within ESI OpenFOAM on current HPC systems like ARCHER2 and produce report and development plan.	Q2 2023
	Implement new linear algebra capability into the MUI coupling library to remove dependency on Eigen and to enable decomposed parallel solutions using the Radial Basis Function spatial filter. Release via GitHub.	Q2 2023
	Implement new coupling scheme helper functionality into the MUI coupling library. Release via GitHub.	Q2 2023
	Create top-level documentation for the MUI library (including new functionality) with the goal of simplifying use for the WSI community. Release via GitHub.	Q2 2023
	Redesign the *interFSIFoam* CFD solver in the ParaSiF framework to use the new MUI coupling scheme functionality and integrate with the latest MUI enabled ESI OpenFOAM version. Release via GitHub.	Q2 2023
	Extend ESI OpenFOAM dynamic load balancing library to work with the other moving mesh classes.	Q2 2023
	Organise and deliver a workshop around understanding OpenFOAM parallel performance and execution.	Q2 2023
	Investigate the potential for GPU acceleration of ESI OpenFOAM (following initial works like Petsc4Foam) and produce report and development plan.	Q2 2023
	Redesign the FEniCS based structural solver in the ParaSiF framework to use the new MUI coupling scheme functionality and re-implement using the modern FEniCSx framework. Release via GitHub.	Q3 2023
	Research Object Catalogue Second release: adds software and publications to project and test cases.	Q3 2023
	Utilise the new ParaSiF framework to simulate the upcoming CCP-WSI+ blind test problem.	Q3 2023
	Integrate ParaFEM stand-alone structural solver into ParaSiF framework. Release via GitHub.	Q4 2023

	Integrate capability of CCP-WSI+ solvers into updated interFSIFoam solver. Release via GitHub.	Q4 2023
	Explore HPC coupling on ARCHER2, including high performance Fluid-Fluid/Fluid-Structure coupling algorithms for both single phase and multiple phase	Q4 2023
	Research Object Catalogue Third release: adds events and news.	Q1 2024
	Data Repository development and maintenance. This task continues through the CCP's life and is therefore carried forward.	Q1 2024
	Website and Software Catalogue development and maintenance. This task continues through the CCP's life and is therefore carried forward.	Q1 2024

HEC-WSI	Milestone	Target Date
	Maintenance and development of website content and features in direct collaboration with Plymouth RSE and admin support	Ongoing
	Provide direct support to HEC-WSI community to enable code running on ARCHER2 and other national systems	Ongoing
	Release first round of access calls, including new web forms	Q2 2023
	Clearly define all data owners and processes to ensure GDPR compliance in access calls, satisfying ARCHER2 and EPSRC trusted research requirements	Q3 2023
	Profiling and benchmarking key OpenFOAM codes on ARCHER2 – providing detailed insight into locations limiting scalability for WSI problems	Q4 2023
	Working directly with Plymouth RSE, help to define and develop key WSI test cases and examples to highlight HPC capability on ARCHER2	Q4 2023
	Integrate and report on CCP-WSI+ dynamic load balancing capability into generic FOAM solvers used by the WSI community on ARCHER2	Q1 2024
	Use detailed profiling and outputs from key projects like exaFOAM to improve scalability and applicability for the interFoam OpenFOAM solver on ARCHER2 for WSI problems	Q2 2024

CCP NTH	Milestone	Target Date
	~~To add multiphase flow simulation capability into CHAPSim2~~	~~Q4 2023~~
	Launch of CHAPSim2 with cylindrical coordinates	Q1 2024

UKTC	Milestone	Target Date
	To be confirmed following the HEC call announcement	

CCP Turbulence	Milestone	Target Date
	Initial porting of X3div developments to the new X3d2	Q3 2023
	Publication work on Lagragian particle tracking in Xcompact3d	Q4 2023
	Publication work for 2decompt&FFT and x3div (ParCFD2023 / SC23)	Q4 2023
	Initial porting of the 2decomp&FFT library to AMD GPU adapting the code already available for NVIDIA	Q1 2024

Tomographic Imaging

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives	Ongoing
	Organise executive committee and working group meetings, as well as monthly show-and-tell sessions	Ongoing
	Support current training courses and organise developer workshops. Assist in new proposal writing.	Ongoing
	Embed lab-based framework: UoM/ UoS/ UoW	Ongoing
	Code integration with CCPPETMR	Ongoing
	Further development of CIL with priorities set with the CCPi executive/steering panel	Ongoing
	Collaboration with Manchester and ESRF. Provide reconstruction capability at ESRF	Ongoing
	Collaboration: Working with Brian Bay (USA) on improving and enhancing the digital volume correlation code	Ongoing
	Release of the digital volume correlation code and distributing it to CCPi community.	Q2 2023
	Release of simplified optimised reconstructor routines for cone beam and parallel beam CT in CIL, including FDK and iterative reconstruction with regularisation	
	Publication of a scientific article based on work enabled by CCPi Digital Volume Correlation	

	Investigation of ML/AI methods for tomography	
	Providing support for iterative reconstruction at facilities CLF/EPAC	
	Development of tools for GUI and interaction/visualisation of scientific data (CILViewer)	

CCPSyneRBI	Milestone	Target Date
	Extended SPECT support (via STIR).	Q2 2023
	Reconstruction pipelines for static data (via XNAT).	Q2 2023
	Conda install of SIRF	Q3 2023
	Joint motion and reconstruction estimation (with CIL).	Q3 2023
	Complete integration of Time-of-Flight capabilities of STIR	Q3 2023
	LPS coordinate system handling.	Q4 2023
	Error checks for input.	Q1 2024
	More extensive and systematic testing.	Q1 2024
	Further code optimization.	Q1 2024

Quantum Computing

CCP-QC	Milestone	Target Date
	Setup new WG Condensed matter	Q2 2023
	Management Board meeting	Q3 2023
	Workshop on QM and Condensed Matter	Q3 2023
	Identify new working package for last year of CCP-QC	Q4 2023
	Management Board meeting	Q1 2024

Appendix 3 – Code Development 2022-23

This appendix contains updates on code developments during 2022-23.

Materials Science

CCP9	Code Development	Comments
W90	• type definition and classification • error handling • library interface • documentation/testing	• complete • complete • complete • ongoing
QUESTAAL	Spin-dependent susceptibilities in BSE	Ongoing
ONETEP	• stress-tensor & optimization of the unit-cell parameters • read pseudopotentials in UPF file format	• complete • ongoing
CRYSTAL	New release: CRYSTAL23	complete

CCPNC	Code Development	Comments
Soprano	• New documentation website structure • Command-line interface structure added (some common NMR workflows implemented)	• Complete • Complete (beta-version)
SODORG Python (New code developed to treat disordered molecular crystals.)	• Parse CIF files containing disorder tags • Generate all possible ordered structures for a given supercell size. • Merge symmetry-equivalent configurations • Handle Z < 1 cases • Perform thermodynamic analysis • Write documentation	• Complete • Complete • Complete • Ongoing • Ongoing • Minimal version published.
MagresView 2.0	• Solicit feedback from users on initial release • Improved 1D spectrum plotting • Improved user experience (added tooltips, choice of colour maps, reset options buttons, smarter bonding algorithm etc.) • New Euler angle visualisation tool • Export spin system to e.g. Simpson	• Complete • Comple • Complete • Ongoing • Ongoing

MCC	Code Development	Comments
ChemShell	• Interface to MolSSI basis set library • Tcl-ChemShell and Py-ChemShell central modules made available on ARCHER2	• Complete • Complete
CRYSTAL	Testing and release of CRYSTAL23	Complete

DL_FIELD	• Support for COMPASS force field for general organic molecules • Bio-inorganic/mixed potential model setup: enable auto fitting of Morse to LJ 12-6 potential for vdw mixing. • Release version 4.9 including manual updates	• Complete • Complete • Complete
DL_POLY	General purpose on-the-fly correlator	Complete

Biological Science

CCPBioSim	Code Development	Comments
CodeEntropy	First release	First stable release of new methodology for entropic information from MD simulations
Website	• New branding including logo • Slimmd redesigned to be more streamlined and categorised by type of simulation • All web pages rewritten to focus on a clearer message about the CCP and its purpose.	First version released

HECBioSim	Code Development	Comment
Resource calculator	• Refreshed resource calculator released with energy model for net zero. • Added new data models for sulis and wilkes3. • Work is in progress to fix bug reported in ARCHER2 model.	

Computational Engineering

UK-COMES	Code Development	Comment
DL_MESO	• PLUMED interface for DPD code to enable free-energy calculations, enhanced sampling and analyses • Trajectory file writing in netCDF format • Improved input file reading and restart file writing in LBE code	• Complete • Complete • Complete
HiLeMMS	• High-level abstractions designed for writing user applications and integrating user contributions.	• Complete

	• Free surface flow capability added into HiLeMMS/MPLB	• Complete

CCP-WSI+	Code Development		Comments
Research Object Catalogue	Software	Development to CCP-WSI+ requirements: 1. Re-evaluate Framework	 1. In progress
	Admin	1. Updates for first release 2. Improve icons 3. First Release 4. Additional resources added for second release	1. Complete 2. Complete 3. Complete 4. In progress
	Projects and Test Cases	1. Additions to schemas 2. Related entries linked 3. First Release	1. Complete 2. Complete 3. Complete
	Publications	1. Schema	1. In progress
ParaSiF	1. Release as open source on GitHub 2. Port and compiled on ARCHER2 3. Port and compiled on SCARF 4. Integrate MUI into latest ESI OpenFOAM 5. Release MUI integration publicly 6. Redesign *interFSIFoam* solver from ParaSiF for latest ESI OpenFOAM release 7. Update FEniCS structural solver to FEniCSx 8. Add additional structural modelling capability to structural solver for thin membrane problems 9. Integrate harmonised CCP-WSI *interFoam* solver into redesigned *interFSIFoam* solver		1. Complete 2. Complete 3. Complete 4. Complete 5. In-progress 6. Complete 7. In-progress 8. In-progress 9. Pending
ParaFEM	1. Define requirements for stand-alone solver 2. Create new solver based on latest ParaFEM 3. Package ParaFEM using Spack 4. Integrate new solver into ParaSiF		1. Complete 2. On hold (resourcing) 3. On hold (resourcing) 4. On-hold (resourcing)
Multiscale Universal Interface code coupling library	1. Maintain and support library 2. Develop parallel performance of library for use on highly parallel architectures like ARCHER2 3. Integrate the library fundamentally into ESI OpenFOAM 4. Add new coupling scheme helper functionality for WSI problems 5. Add new stand-alone linear algebra capability 6. Integrate new linear algebra library into Radial Basis Function spatial filter to enable decomposed parallel problems 7. Performance optimise new linear algebra library		1. Ongoing 2. Complete 3. Complete 4. Complete 5. Complete 6. Complete 7. In-progress

ccp-wsi Repository	1. Improve code maintainability by removing redundant code 2. Restructure the code for the latest ESI OpenFOAM releases 3. Expand to include future code releases (ParaSiF integrations) and other related software 4. DLB and new OpenFOAM fluid apps with GPU capability	1. Complete 2. Complete 3. In-progress
decomposePar (ParMETIS based)	1. Create as stand-alone library/application (rather than patch for specific OpenFOAM versions) 2. Integrate into latest ESI versions and release via repository	1. Complete 2. In-progress
ESI OpenFOAM load-balancing capability	1. Create first instance of new ESI OpenFOAM Class 2. Refine and further develop for general use and addition to latest ESI versions	1. Complete 2. In-progress

CCP NTH	Code Development	Comment
The library 2DECOMP&FFT	Implementing the 3-D sine/cosine Transformation (based on FFTW3) to the library of 2decomp&fft	Complete
CHAPSim2.0	1. Implementing a pre-/post-processing procedure to handle staggered grid in the Poisson solver. 2. Implementing a sine/cosine Transformation in the code for various boundary conditions in the Poisson solver 3. Added Paraview compatible format ‘xdml’ for data output including raw data and space/time averaged data 4. Carrying out performance of CHAPSim2 in Archer2 5. Implementing the cylindrical coordinates to CHAPSim2 for pipe or annular flow simulation 6. Support the development of immersed boundary conditions for CHAPSim2 7. Support the development of multiphase flow simulation in CHAPSim2.	1. Complete 2. Complete 3. Complete 4. Complete 5. Ongoing 6. Ongoing 7. Ongoing

UKCTRF	Code Development	Comment
SENGA 2	• Lines are added in the relevant subroutines to collect boundary information. New boundary conditions are implemented in the subroutine bounds. • Derivation of the full 3D boundary conditions has been completed.	Essential to being implemented into the code

UKTC	Code Development	Comment
	No code development activities	

CCP Turbulence	Code Development	Comment
OPS	• Features for writing out arbitrary section of the computational domain into disk. • Features for writing out data in various precision and reducing the data size for direct numerical simulations.	• Complete • Complete
Xcompact3d	• Release of an independent version of 2decomp&FFT library with both CUDA-aware MPI, NCCL and cuFFT features. https://github.com/xcompact3d/2decomp-fft • Full Navier-Stokes solver for the TGV case fully ported to GPU https://github.com/rfj82982/x3div/tree/TGV_MemManual_DC • First full development version with Lagrangian particle tracking https://github.com/rfj82982/Incompact3d/tree/dev-stfc-particle	• Complete • First scalability studies presented CIUK 2022 • Complete
OpenSBLI	• A python code generator developed for creating implicit solvers based on OpenSBLI • A workflow system is developed for setting up working environment in desktop, ARCHER2, CIRRUS at EPCC, IRIDIS5 at the University of Southampton.	• Complete • First version support GNU compiler is completed

Tomographic Imaging

CCPi	Code Development	Comments
CIL	1. Reader for ZEISS lab X-Ray CT machine, with support for parallel/cone beam geometry as well as TXM file format. 2. Enhanced support for NIKON files to parse and set up geometry with: ObjectTilt CentreOfRotationTop and CentreOfRotationBottom 3. Optimisation framework: added strongly convex functionality in TotalVariation and FGP_TV Functions, new ISTA algorithm	
CIL-ASTRA	Code relicensing from GPL3 to Apache-v2 and subsequent merger into CIL	

CILViewer	New readers for multiple format allowing resampling and cropping while reading. Refactoring of code, with creation of base classes.	

CCPSyneRBI	Code Development	Comments
SIRF	• Add MR acquisition models for 2D non-cartesian encoding. • Add conjugation methods to DataContainer class. • Export a CMake config file such that external C++ projects can use SIRF via CMake. • Generate simulated MR data to be used in tests during the build step to make it compatible with the installed ISMRMRD version. • Ensure compatibility of Python and C++ integers. • Add SPECT acquisition model. • Add support for spiral MR trajectories pre-computed by the user. • Enable writing MR images to files in DICOM format. • Fix MR image processing chains. • Support Gadgetron master of the end of November 2022 on Virtual Machine. • Support Pinhole SPECT. • Support extraction of acquisition data subsets.	• Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete

Atomic and Molecular Physics / Plasma Physics

UK-AMOR	Code Development	Comments
RMAT_REACT	Over the course of UK-AMOR, develop a bound state code (and possibly a resonance code) for low temperature atom-atom (molecule-molecule) reactive collisions, adapting existing code from the electron-molecule UKRMol(+) package and the TIMEDELn time-delay package. *Initial interfacing work for data transfer, as adapted for collision code PFARM, for the preferred bound state code has been examined and adapted for rearrangement channels as part of the Graduate project (supported by MP) in September-March (and in preparation for the planned EPSRC grant antimatter work).*	The Graduate project (ended March 2022) investigated the mixed coordinate systems needed for the R-matrix (bound and quasi-bound) inner region and links to the separate coordinate systems for each arrangement outer region on the boundary hypersurface. A code for numerical integrals transforming between coordinates (with correct inner integral limits) was written as part of the project and

		has undergone further testing (validation/verification) in this reporting period. Additional work on coordinate transformations at DL and on basis states describing protonium proton bound states and resonances at Aberdeen (with some analysis at DL) has taken place.
RMT	Following the ARCHER2 eCSE project, further test the new outer region channel parallelization across a wider range of legacy and large-scale new cases, ready for production use in ~Q1 2023 onwards (ideally earlier). Produce further data indicating the balance of core counts to be used in the highly distinct inner and outer regions of the code.	Complete. The eCSE project introduced new parallel felibility into RMT's inner region coding which can greatly enhanced performance. It also introduced a new parallelization across outer region channels, adding more flexibility (and performance gains for larger cases) to an existing fairly simple targeted OpenMP parallelization and a procedure to distribute MPI tasks optimally between the two regions for best performance. [Note: further improvement possibilities have arisen as a results of this work and will be carried out outside of CoSeC support which officially ended on 31 December 2022.]

Appendix 4 – Training and Outreach 2022-23

This appendix contains updates on training and outreach activities during 2021-22.

Materials Science

CCP9

- "4th QUESTAAL school" at Daresbury Laboratory, 10-13 May 2022. Jerome Jackson organized and tutored at the school.
- "Daresbury DFTB+ school" organized at Daresbury, 6-10 June 2022. Leon Petit was local organizer.
- "MSSC2022-Virtual Ab-initio Modelling in Solid State Chemistry", online 19-23 September 2022. Barry Searle was tutoring at the course.
- "Psi-k Conference", 22-25 August 2022, Lausanne. Posters presented:
- Jerome Jackson: "Electronic structure and finite temperature magnetism of yttrium iron garnet"
- Jerome Jackson: "QSGW+QSGWBSE implementation in the Questaal project"
- Manuel dos Santos Dias: "Global mapping approach to chiral multi-site interactions"
- "Wannier90 as a library", talk given at Psi-k conference: Arash Mostofi, Jerome Jackson, Barry Searle, Leon Petit, Martin Plummer, Giovanni Pizzi, and Jonathan Yates co-authors.
- "CCP5 Summer school", 17-28 July 2022. Barry Searle gave 2 lectures at the school's advanced course on first principles calculations.
- "DPG Spring meeting", 4-9 September 2022, Manuel dos Santos Dias presented a talk entitled "Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3".
- "Wannier90 developers meeting", 23-27 May 2022 ICPT Trieste. Jerome Jackson presented a talk on "Wannier90 library developments".
- July/August, student (JingJing Li) tutoring in DFT and Quantum Espresso by Manuel dos Santos Dias, Jerome Jackson, and Barry Searle
- CCP9 Community meeting Crowne Plaza, Manchester, 7-9 September 2022. Organized by the CCP9 team. Jerome Jackson and Barry Searle presented the ongoing CoSeC work on the QUESTAAL code and the Wannier90 library respectively.
- Jerome Jackson gave an invited talk at the University of Leeds, Department of Physics on the Questaal project 28/11/2022.

CCPNC

The new online discussion meeting series, CCP-NC Online, has had three engaging meetings so far, with two further meetings planned over the coming months. These meetings are a very effective way of engaging with new and existing members of the community. We have also gained insight into issues and interests of the community that allow us to focus our software and science support efforts.

The CCP-NC was also involved in the annual CASTEP Workshop, allowing us to engage directly with new users' issues and interests and providing training in computational methods relevant for the solid-state NMR community.

The documentation website for Soprano – the core CCP-NC Python library – was redeveloped, allowing users to interactively run the tutorials in the cloud (without the need to install anything), thus lowering the barrier-to-entry.

We have also written documentation and tutorials for the new transition state searching method in CASTEP that was previously developed by CoSeC staff.

UKCP

The annual CASTEP teaching workshop was held in Oxford, September 2022, with join support from UKCP and CCP-NC. Unfortunately, Dominik Jochym was unavailable due to illness. Please see CCP-NC section for more details.

MCC

- Ian Bush and Barry Searle gave lectures and tutorials as part of the online CRYSTAL training week MSSC - Ab initio Modelling in Solid State Chemistry, 19-23 September 2022.
- Ilian Todorov organised and opened the "Catalysis for Europe's Green Transition: Advancing industrial catalysis by synergy of experiments and supercomputing simulations" event, 21-24 November 2022, in Sofia, Bulgaria. Co-founded by PRACE, where as part of HEC-MCC Richard Catlow presented, and Tom Keal and Kakali Sen gave an overview of ChemShell driven research and software development.

Biological Science

CCPBioSim

The CCPBioSim Training Week took place from 20-23 September 2022. It was a hybrid event with 23 participants registered to attend in Leeds and 40 participants registered to attend online via Zoom. The varied workshop sessions covered different tools (BioSimSpace, Flare, AutoDock) and simulation scales from electronic structure (QM/MM, BigDFT) to coarse-grained (oxDNA) and elastic network models (ProDy). Cresset Software Company sponsored a networking dinner. Unfortunately, because of the short notice bank holiday we had to cancel the python programming workshop which was scheduled for 19 September 2022. The rest of the week ran smoothly.

HECBioSim

The HEC does not have its own training programme and efforts focus on one to one training via the support route and publishing materials on our website. However, work is proceeding to develop a set of courses that can be delivered as part of the CCP programme that will focus on the basics of simulation on different platforms through to more advanced topics on high level performance. This is expected to be ready in the next grant cycle if the HEC is successfully renewed.

Computational Engineering

UK-COMES

Michael Seaton contributed to the CCP5 Summer School in July 2022 held at Durham University, providing seminar talks on DPD and practical exercises for both DPD and LBE using DL_MESO to 10 students. He also delivered an invited seminar talk at the University of Lincoln on 8th February 2023: "Mesoscale, molecules and more: simulations with DL_Software". He is contributing further training material to the DL_Software Digital Guide (https://dl-sdg.github.io/).

Jianping Meng presented an invited talk (High level discrete Boltzmann modelling system and its applications) at the Discrete Simulation of Fluid Dynamics hybrid conference held at Soochow University in China and online in August 2022. He also presented two invited talks, one at the University of Birmingham on 9th November 2022 – "Domain-specific language for exascale lattice Boltzmann simulations" – and one at the University of Hull on 23rd February 2023 ("Multiscale simulation of the multiphase fluid dynamics using exascale supercomputer").

CCP-WSI+

No events during this reporting period.

CCP-NTH

During this report period, CCP-NTH organed/co-organized below training course / workshops to support the CCP-NTH community development and increase impact of CoSeC on university research. (1) A training course "HPC for CFD using Code_Saturne" was held on 27-28 April 2022 online. This course was organised by CCP-NTH/UKTC in association with ARCHER2 and PRACE. The open-source HPC software Code_Saturne was used by the participants to run large scale simulations using the UK national facility ARCHER2. (2) UK developers' meeting on Code_Saturne was held on 30 November 2022 organized by EDF Energy, CCP-NTH/UKTC and Manchester university. There were 28 participants to share experiences in Code_Saturne development and applications. (3) CCP-NTH workshop was held in November on CHAPSim2 development. The majority of CHAPSim2 users in the UK attended to discuss the recent development of CHAPSim2 and their application of it.

During this report period, CCP-NTH organized/attended various events for outreach. These includes: (1) The 2022 Annual Technical Meeting of CCP-NTH and the SIG-NTH meeting were held by CCP-NTH on 27-28 June 2022 in Cambridge University. The Technical Meeting comprised an update on the CCP-NTH, followed by a keynote talk, and short and extended presentations from the community. Over 40 participants attended this meeting, including international collaborators from both industry and academia. (2) A few members of CCP-NTH attended the UK fluid conference held at the University of Sheffield on 6-8 September and presented recent results on thermal-hydraulic related topics. These include a talk from myself, and a poster from a PDRA co-supervised by me. (3) A few members of CCP-NTH attended and presented in the CoSeC Annual Conference and Computing Insight UK – Sustainable HPC, 1-2 December, 2022. (4) CCP-NTH and CCP-Turbulence keeps close contact, especially in the development and application of the 2decomp&FFT libraries. Several cross-CCP events, focusing on that shared library (2decomp&fft) was held regularly. The main code developer of CCP-NTH talked and reported experiences in using 2decomp&fft lib and new development of Sine/Cosine Transformation into this lib, and potential application of 2decomp&fft into cylindrical coordinates. As part of cross-CCP communications, the main code developer of CCP-NTH attended Xcompact3d (one of the main codes of CCP-Turbulence supports) hackathon and shared my thoughts.

Regular weekly meetings and occasional one-to-one meetings were carried out with CHAPSim Users (mainly PhD students from the University of Sheffield and Liverpool John Moores University) to support their use of CHAPSim to their research. These regular weekly meetings strengthen the link between universities and CoSeC researchers, keeps a good track of each other' progress in research and code-development and improves the doctorial training by prompt support from CoSeC researchers. We also support users of Code_Saturne, which mainly come from University of Sheffield and University of Manchester, in their research of nuclear related flow and heat transfer simulation.

CCP-NTH also supports the outreach and the community via distributing members' latest news on seminars, conferences, training and recruitment to all the NTH community.

UKCTRF

The University of Leeds is a member of UKCTRF. Dave Emerson was supervising a Ph.D student in the School of Mechanical Engineering to implement the flametlet model in Code_Saturne along with his supervisors Professor Derek Bradley and Dr Junfeng Yang. The weekly remote meeting was held to train the student and monitor his progress.

Dave has delivered two lectures on the modelling and simulation of turbulent flows for the Ph.D students in the combustion group in the Mechanical Engineering School at the University of Leeds.

UKTC

No training and outreach activities.

CCP Turbulence

A regular hackathon event to bring the Xcompact3d development community together is on-going every 3 months. The event is organised by the CCPTurbulence chair (Dr. S. Laizet) and S. Rolfo, J. Fang and C. Moulinec are regular attendees and contributors. In the first semester events were 27-28 June and 28 September 2022 in the second on 1 December 2022 and on 19 January 2023.

All the member of the CCP-Turbulence were at the centre of the organisation of the ParCFD2022 event in Italy from 25 to 27 May 2022 with around 130 participants form Europe, North America, and Asia. Seven keynote lectures were given including the one from Dr Rupak Biswas from NASA about NASA's vision for quantum computing. 108 contributions covering several aspects of CFD and HPC were presented.

CCP-Turbulence has also organised a Code_Saturne training course for 3 days (19-21 July 2022), together with Politecnico di Torino (Prof. D. Marchisio) and CINECA (Dr. G. Amati). The course was also supported by the Daresbury and IT-Simul CECAM nodes and had about 20 participants from different institutions.

CCP-Turbulence has also organised the UK Code_Saturne development meeting on 30/11/2022 with about 35 participants from both Academia (University of Manchester, University of Sheffield, University of Newcastle) and industry (EDF R&D France and UK, Renuda).

Tomographic Imaging

CCPi

During the reporting period Edoardo Pasca and Evangelos Papoutsellis presented the CCPi Core Imaging Library at 3 international conferences: PyCon DE & PyData Berlin 2022, dimensional X-ray CT (dXCT) 2022 and Tomography for Scientific Advancement (ToScA).

Evangelos Papoutsellis presented the work on CIL that has been carried on stochastic algorithms at the two-day workshop on modern image reconstruction algorithms and practices for medical imaging, concentrating on PET, MRI and CT, sponsored by CCP SyneRBI, held at UCL 12-13 Sept 2022.

Edoardo Pasca presented CIL at:

- Inverse Days (Kuopio, Finland) 16/12/22
- NATO SET-319/RSM New Mathematics for Multi-Dimensional Radar Systems, Edinburgh 21-23 February 2023

During the reporting period the following training events have been organised:

- Online session with 13 trainees (27/04/22)
- 7th annual CINEMAX Summer School on 3D imaging, https://www.conferencemanager.dk/cinemaxvii at Fuglsang Manor 22-26 August 2022
- 2 training sessions at the ToScA conference with 20 trainees in total (07/09/22)
- 1 day training session at the IBSim-4i conference, 20 trainees (18/10/22)
- 1 training day on Digital Volume Correlation at the Diamond Light Source, 6/12/23
- 1 day training session at the Isaac Newton Institute, followed by 2 day Hackathon, Cambridge 20-23 March 2023

The team also supports users by means of the Discord channel, mailing list and via recurring meetings.

CCPSyneRBI

Our main training activity was the training school on SPECT/PET/MR Image Reconstruction on Saturday 28th of May 2022 for the participants of 9th PSMR-TBP Conference on PET/MR and SPECT/MR and TotalBody PET. The in-person course was taken by 25 people, 10 of which left feedback (4.5 stars out of 5 on average). CoSeC provided the training material, access to JupyterHub instances with SIRF and CIL on the STFC Cluster, as well as in-person support during the course.

CCP SyneRBI, together with CCPi, supported the QUIERO Workshop on Cardiac MRF Simulation & Evaluation, held on 6 July 2022, that provided participants with hands-on experience on simulation of MRF data acquisition and evaluation of T1 and T2 maps in clinical practice and using advanced machine learning approaches. CoSeC provided access to JupyterHub instances with SIRF and CIL on the STFC Cluster.

CCP SyneRBI also sponsored a two-day (12-13 Sept 2022) workshop at UCL on modern image reconstruction algorithms and practices for medical imaging, concentrating on PET, MRI and CT. CoSeC provided registration and website support, and Evangelos Papoutselis (CCPi and SyneRBI) gave a talk describing latest progress on the use of CIL with emphasis on stochastic optimisation algorithms.

Atomic and Molecular Physics / Plasma Physics

UK-AMOR

Training activities provided by SLA/CoSeC for UK-AMOR members are generally in the form of specialized informal group meetings and one-to-one interactions (local and virtual). In this reporting period there have been 'scientific code' discussions on various topics. These include the adaptation of RmatReact for antimatter and rearrangement collisions, with particular emphasis on coordinate systems and basis sets, the capabilities of the RMT code with the Queen's University Belfast RMT group, as well as separate discussions on muonic atoms and relativistic collisions using the Dirac equation. [Discussions on multiphoton topics, electron-atom interactions and the RMT code also took place as part of other projects (the eCSE and the AquA-Dip grant) obtained as part of UK-AMOR/CCPQ work,]

Quantum Computing

CCP-QC

Alin Elena was part of the judging panel at National Quantum Computing Hackaton week July 2022 at Royal Holloway University London.

Jianping Meng undertook the QC work on work package 4 from CoSeC side.

Scientific Applications of Quantum Computing: Materials, Chemistry and Biology - September 2023 workshop is in preparation, this will be in collaboration with other projects like MCC and QVEC.

Phalgun Lolur from NQCC, hosted at Daresbury Laboratory and delivered a community talk about Quantum Computing for Chemistry and Materials Science: Resource Estimation and Outlook.