Computational Science Centre for Research Communities

Financial Year 2023-2024 Annual Report

(*Covering the period 1 April 2023 – 31 March 2024*)

Contents

Figures, Tables and Graphs

1. Executive Summary 2023-24

CoSeC 2027: Over the course of this reporting year, EPSRC and CoSeC have held discussions around the strategic future of the programme considering the continuing success around the wider UKRI Digital Research Infrastructure (DRI) programme. As part of this, EPSRC (and all research councils) are aligning relevant parts of their individual DRI strategies with the wider UKRI one. In the final quarter of this year, consultation with the CoSeC Steering Committee began around a proposed change in model, with CoSeC becoming funded directly by the UKRI DRI programme alongside continued strategic investment by EPSRC, BBSRC and MRC. This was discussed at length with both the Steering Committee and then more widely with CoSeC's Steering Panel (that includes all Chairs of currently funded communities) with a view to putting the change into action during 2024 – 2025.

Resources: Programme resources for 2023 – 2024 can be seen in detail in Section 4, the available staffing levels the direct funding from EPSRC enables remain largely static compared to the previous year, with a slight uplift of 0.5 FTE for the Programme Office and a further 0.3 FTE enabled within the community support envelope. This additional effort is found through minimal cost increase to EPSRC (with the high-level costing remaining within the prior fixed £2.2m envelope of recent years) as well as offsetting staff cost increases due to career progression or UKRI pay increases through internal STFC funding. It is notable that this offsetting is possible for this reporting year only due to the exceptional nature of STFC's pay reforms, in future years, increased staff costs will reflect in reduced overall staff effort given a fixed funding envelope, as with previous years.

Both CCP4 and CCP-EM remain funded independently through BBSRC and MRC, with their CoSeC Core Support delivered as an integrated element of their respective grants. Figures related to this are not reflected directly in this report, where EPSRC funding is shown but objectives and outcomes related to these communities remain an integrated element of CoSeC, ensuring cross-fertilisation between the funded communities regardless of which council supports them.

Large-scale Computing: CoSeC technical staff continue to work synergistically with key national efforts around large-scale computing. Notably, a number of CoSeC Project Leaders are also directly involved in the delivery of projects funded through the ExCALIBUR programme and success within Scientific Computing around the eCSE programme of funding remains high.

The ExCALIBUR projects reported in 2022 – 2023 remain ongoing, with key codes from across the CCPs and HECs under development towards the use of exascale supercomputers, including: xCompact3d (CCP Turbulence, UKTC); the Multiscale Universal Interface code coupling library (CCP-WSI, HEC-WSI); CASTEP (CCP9, UKCP, CCP-NC, MCC); 2DECOMP&FFT (CCP Turbulence, UKTC, CCP-NTH).

The High-end Computing Consortia supported by CoSeC remain a key element of the EPSRC strategy for use of its supercomputing resources, with CoSeC staff playing a key role in helping to orchestrate the resources that the HECs hold. many of these communities are now mature and hugely effective in terms of their processes. In the case of newer communities such as HEC-WSI, CoSeC has provided key input to ensure efficient and useful delivery of held resources to the wider community. Across all HECs, CoSeC staff remain integral to the development, delivery and maintenance of key simulation and related enabling software.

Data Infrastructure: As a programme involving Scientific Computing, the Physical Sciences Data Infrastructure (PSDI) programme remains a key partner for CoSeC when considering strategy related to delivery of national data infrastructure. Work through bio-simulation communities has continued with development of the PSDI pathfinder related to the use of AiiDA demonstrated within CCP-EM.

Software: A detailed overview of activities related to the development of community software can be found in the appendices of this document. During this reporting period there have been notable releases, developments and strategies devised across the communities related to the research software at their core. Within CCP-WSI, the Multiscale Universal Interface (MUI) code coupling library had a major 2.0 release with many of the changes driven by the needs of the community. The ParaSiF multi-physics simulation framework also saw development, with its finite-element structural solver being redeveloped around the FEniCSx framework.

The UKCOMES community facilitated a new release of the DL_MESO software package, which adds new capability related to the use of Dissipative Particle Dynamics (DPD) and the Lattice-Boltzmann (LBE) method. Alongside this, CCP-NTH developed the CHAPSim2 package in a number of ways driven by community need related to pre and post processing, data visualisation capability and understanding large-scale computing performance.

Within UKTC and CCP Turbulence key developments of the 2DECOMP&FFT library were made, including development of GPU capability. This underlying library was a key part of a new release of the Xcompact3d software, resulting in GPU capability there also.

The Core Imaging Library (CIL) was further developed within CCPi, enabling support for new x-ray machines and data types, a new 3D viewer called CILViewer was also developed and released. There were two releases of the SiRF package by CCPSyneRBI during this reporting period. The first of these, 3.5, saw a fundamental change in the replacement of underlying Python code for more performant C++, the second, 3.6, saw a large number of new capabilities added.

CCP9 completed the process of redeveloping Wannier90 into a library and are now looking at this in terms of parallel performance. This will enable the use of Wannier90 through other code interfaces, increasing the availability to a wider part of the community. Amongst many other developments within CCP9, the QUESTALL software received new additions to further support community needs. The 23.1 release of CASTEP was driven by UKCP as well as a public beta release of the GPU version of CASTEP. The community improved the continuous integration (CI) capabilities of the CASTEP repositories to enable multiple build systems and improve code maintainability.

Within CCPNC there was development of workflows from the Galaxy platform's management tools so they now support the CCPNC NMR post-processing tools, opening up new capability within the community. Within MCC, CRYSTAL23 was deployed on the latest Archer2 software stack and development of a new interoperability layer for CP2K was also started. The DL_FIELD software was extended to handle CHARMM format files, increasing compatibility and community capability.

Within CCPBioSim and HECBioSim there have been a number of incremental developments to key software packages, including important but tricky bug fixes. A focus was placed on CodeEntropy, which has received development efforts and skilled staff have been identified and are in the process of being deployed within the respective communities to enable further key developments during the next reporting period.

Training: Highlights of the year included the 2023 MCC conference that was hosted at Daresbury Laboratory, 28-30 June, UKCPs annual CASTEP teaching workshop that was held in York, September 2023, the CCPBioSim Training week in Leeds, 25 – 29 September 2023 and the ongoing discussion meeting series, CCP-NC Online, that has had five meetings to date, with the most popular (109 participants with 58% participation from academic institutions and companies from outside the UK) of these occurring during this reporting period. In total the programme has provided 1939 training days during financial year 2023-24.

Forward Strategy: The upcoming investment into CoSeC by the UKRI DRI programme will begin during the next reporting period. Over the course of 2024 – 2025 a new programme office will be created within Scientific Computing including a full time Director, Programme Manager, administration support, part time research community manager and part time events organiser. CoSeC will also take on the role of funder, providing a key opportunity for currently funded CCPs and an open call to create new communities from across all of UKRI's council areas. As part of this, CoSeC will reposition itself so that it maintains the integrated technical (core) support role it currently has, while also helping to provide strategic guidance and support to the communities that it will fund. It will do this in close collaboration with colleagues across UKRI in EPSRC, BBSRC and MRC, with potential that this will widen to other council areas as result of the open call for new communities.

This change will see the oversight model of CoSeC evolve with the EPSRC Steering Committee reaching a natural conclusion and new methods such as the CoSeC Community Forum (an evolution of the Steering Panel), an external advisory board and UKRI oversight instead taking its place. A result of this will be that these reports will no longer be generated in this format, instead CoSeC will curate metrics and outcomes through reports created for the Community Forum as well as official reporting submitted through awarded grants. It will continue to gather metrics internally, with a view to publishing these annually alongside a portfolio of impact reports.

2. Impact 2023-24

In this section we highlight some areas where the work of CoSeC during this reporting period (1 April 2023 – 31 March 2024) is having an impact in our communities, across our communities and further into the general public domain.

The 2023 CoSeC Impact Award

Now in its fourth 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.

The winner of the 2023 Award was **Iwan Mitchell from Bangor University** for his research into producing digital twins of industrial x-ray scanners - **Congratulations!**

Overview of the Research

X-ray Computed Tomography (XCT) produces 3D images of the interior of objects without damage. To "reconstruct" a CT image, thousands of X-ray images must be taken. It is widely used in medicine for the diagnostics of pathologies. Similarly, XCT is used in critical industries to ensure manufactured parts

have no internal defects. In the past, computerised X-ray simulation required particle simulation via Monte-Carlo methods. Although accurate, these take hours for each image, and months to simulate enough images for a tomographic reconstruction. Using a GPU-based method, gVirtualXRay (gVXR) is an open-source X-ray simulator able to create enough accurate images for a full dataset within seconds. Most reconstruction software is proprietary, making access difficult for the scientific community, especially those without X-ray scanners. CCPi's Core Imaging Library (CIL) provides an open API for many reconstruction methods, including the building blocks for cutting-edge research regarding new techniques. However, it is aimed at Python developers. I aim to recreate X-ray scanners virtually; including behaviours and defects pure physics-based simulators fail to accommodate. These Digital Twins of real scanners can be used for planning acquisitions before being on-site, providing training to users without physical samples and beamtime, and creating large datasets for defect-detecting machine learning algorithms. CIL has been essential in my work on WebCT: a user-friendly and open-source browser-based X-ray simulation and reconstruction software, to make scan planning and training on X-ray CT accessible to those without extensive Python and X-ray CT knowledge. Support and expertise from the CIL team via in-person workshops and discussions on the CIL community discord has assisted greatly with tight integration. I've been invited to a CCPi working group meeting at the STFC Harwell Campus to present WebCT and discuss the use of scan planning to save time at beamlines such as Diamond Light Source.

Impact of the Research

Iwan's research into producing Digital Twins of industrial XCT scanners has resulted in the ability to simulate X-ray images in gVXR and reconstruct CT volumes with CCPi's CIL, resulting in the first fully open-source virtual NDT workflow from sample to measurements. Due to the virtual nature of this workflow, the bar of entry into the X-ray NDT field is minimised, previously requiring very expensive hardware, and inaccessible proprietary software. A large amount of time during X-ray scanning is wasted by feasibility questions, and tweaking parameters to optimise the scan quality. For most scientists in the UK, proposals are required to get access to an X-ray facility (e.g. from NXCT or the Diamond Light Source), and maximising data acquisition in the limited allotted time is critical. My project WebCT aims to solve this issue by providing an accessible interface while being easy to learn. Researchers can learn the basics of X-ray NDT by changing parameters such as voltage, amperage, and filtration, seeing their virtual scanner produce images in real time. This allows them to discover if their sample is unsuitable, or what resolution and imaging artefacts they will receive from a real scan. WebCT also exposes many aspects of CCPi's CIL, such as cutting-edge reconstruction regularisers, along with high-performance tomographic reconstruction.WebCT has been presented in the IBSim-4i 2022 Image-Based Simulation for Industry conference, awarded Best Poster at the Dimensional X-ray Computed Tomography 2022 conference, and presented as part of a discussion on simulation for machine learning optimisation methods at the Workshop on Korea-UK AI/ML Research in Fundamental Sciences at Sejong University, Seoul. Impact is not limited to training and feasibility questions. Current research into using Machine Learning methods to optimise manufacturing design, require very large datasets and cannot be trained without X-ray simulations. Existing methods for accurate simulations are very slow and fail to provide the data quantity training models require. The use of Digital Twins with gVXR can produce a tomographic dataset in seconds, opening the gateway and closing the loop for Machine Learning. This has already been applied with CIL to simulate defects in surrogate nuclear fuel pellets, and has successfully identified issues in manufacturing, such as unexpected porosity and internal cracks. In addition to defect detection, and manufacturing optimisation, work is ongoing to apply Machine Learning for optimising the scanning system itself; by adjusting X-ray tube and detector parameters for a given sample to minimise imaging artefacts. This is a work in progress, however a large impact in academics and industry is expected, dramatically

simplifying the pre-processing work for NDT experts. Optimising the image quality offline is becoming possible, leading to better and cheaper scans, and an improve public safety in general if the detectability of defects can be maximised in a consistent and systematic manner.

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

During 2024/25 major efforts will be devoted to linking the W90 library to a number of codes, for example CASTEP and CRYSTAL, as well as implementing DMFT in CASTEP.

CCPNC

In the 2024-2025 period, our goal will be to release "2.0" versions of various projects, including our Python library, Soprano, our repository of computed NMR data and MagresView (WP1.1a). These major releases will aim to significantly enhance the user (and to some extent developer) experience.

In addition, we plan to release our code that tackles disorder in molecular crystals in the form of a publication, together with a case study run in collaboration with the Cambridge Crystallographic Data Centre (CCDC).

The work on CCP-NC database has commenced and ongoing. The major developments for introducing more complex search features to the existing database, incorporating a large dataset from the ShiftML2 training data, and rebuilding the CCP-NC database software stack replacing the deprecated AngularJS framework carries forward into the 2024-25 period.

Following our expansion of user engagement activities (WP2.1–WP2.3), we will continue to run the CCP-NC Online meeting series. The Faraday Discussion meeting on NMR Crystallography is planned for September 2024 and will allow for in-depth discussions of emerging computational and experimental methods in the field of NMR crystallography, as well as the current limitations and challenges that need to be overcome to broaden applications to increasingly complex materials.

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 continue the development and deployment of a web service for CASTEP licensee queries (delayed from 22/23). 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 software development project will be determined and carried out that will bring added value in scientific capability of CASTEP to the UKCP and wider CASTEP user communities.

MCC

Ab initio DFT development activities will expand to support CP2K as well as CRYSTAL, through developing interoperability for basis set and density matrix data between the two codes, so enabling users to more easily switch between them. The new MCC CoSeC focus on ML methods will continue with benchmarking of ML IPs for diffusion in zeolites, taking forward the methods previously used to look at MOFs (which will also be further fine tuned). Core development in DL_FIELD will continue with

support for new file formats from GROMACS and new forcefields for complex inorganic systems. A community training/user workshop will be organised for DL_POLY. ChemShell development will focus on advanced microiterative optimisation techniques, new QM/MM embedding functionality and integration of ML approaches for geometry optimisation and interatomic potentials.

Biological Science

CCPBioSim

In 2024/25 we will work on software projects relating to the setup and analysis of biomolecular systems. The CodeEntropy project will continue to be developed and maintained with work on entropy of mixtures and improving documentation. We will collaborate with experimentalists (for example colleagues at ISIS) wherever possible. CCPBioSim's training and networking activities will as always be an important part of our work.

HECBioSim

The 2024/25 plans are as follows. The PDRA has now been appointed at Oxford for the ML/AI project so the project is starting in earnest April 2024. The plans for the 24/25 year will contain a large element of ongoing support for the consortium and its research 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 continue on from last years efforts and further develop a series of HPC focused course for biomolecular simulation. The ExaBioSim ExCALIBUR project is working on extending our benchmarking suite and we will work on incorporating that into our standard set as well as use them to enable more research groups to benefit from our resource calculator. We have seen an uptick in the use of codes we currently do not benchmark in the HPC time requests, so we will look to understand how these operate and expand our understanding of hardware platforms most suitable for them. We are re-establishing the HECBioSim software development activity and it will focus on the development of high performance applications for simulation across our HPC landscape.

Computational Engineering

UK-COMES

Interfaces in both the DPD and LBE codes of DL_MESO 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.

An interface in the LBE code of DL_MESO for AMReX will be created to enable adaptive mesh refinement and multi-resolution LBE calculations. The ability to refine a lattice close to obstacles or other features in a flow-based system will provide greater accuracy in an LBE simulation where it is needed and allow for coarse lattices elsewhere, significantly speeding up the calculation.

CCP-WSI+

With a well-defined software strategy now in place for the WSI community, the goals and outputs over the 24/25 period are clear. By the end of this period the intention is for the ParaSiF framework to be a robust, capable and accessible software resource the for WSI community for the fluid, structural and coupled FSI components of the FOWT problem, over this time other projects and collaborations will be used to further extend this, introducing other physical capabilities like soil mechanics and flexible tethering.

The underlying MUI coupling technology developed by CoSeC will be generally included in the OpenFOAM framework, simplifying its use not only for the WSI community but also for the FOAM community as a whole. The ability to couple OpenFOAM overset mesh with a solid mechanics solver will be developed. A particular focus is to build a coupled FOWT test case using overset mesh coupled with solids4Foam The on-going work around 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. Through feedback of the previously released resource types we are learning how to improve its potential impact and are making links with other catalogue providers in STFC to the benefit of all.

HEC-WSI

The first 12 months of the HEC are focussed on ensuring it can deliver its basic function – to be a gateway to national computing infrastructure for the WSI community. During this time, exploratory work will also happen to define where focus should be paid in terms of the key codes used by the WSI community, with initial attention on the interFoam solver from OpenFOAM. During 24/25, the potential for improving the performance, scalability and portability of interFoam based solutions will begin and will be undertaken in close collaboration with those also considering this such as ESI and others currently involved in the exaFOAM project.

We also started to look into the porting to OpenFOAM on GPU accelerators starting from PETSc4FOAM and defining a sustainable and portable strategy (mainly based on modern C++) which will allow to offload OpenFOAM on any GPU vendor hardware.

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 main activity for the CCP Turbulence will be related to the build of a multi targets version of 2DECOMp&FFT library to support different back-ends for different architectures. This will be achieved using a more object-oriented programming in modern Fortran and will create a more flexible structure to allow the inclusion of different backends that are necessary as the evolution of heterogeneous HPC hardware progress and vendors put new products on the market. The work will first start by creating a MPI backend to support traditional application, CUDA Fortran backend for NVIDIA GPU and an OpenMP offload for others GPU. Additionally, we aim to provide support for the enhancement of OPS software in terms of Continuous Integration/Continuous Deployment (CI/CD) practices.

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 2024/25 we plan to provide example interfaces to Machine Learning frameworks and design the strategy for developing new functionality and interface. We will also provide additional support for measured data and dynamic/gated data with parametric models, and we will further our code optimization efforts.

Quantum Computing

CCP-QC

Quantum computing and condensed matter have a long common history, the new established working group will look into possible synergies for quantum computing and post dft methods, as GW. A series of informal meetings will be planned with a more formal workshop to happen in Q2/2024 in collaboraiton with NPL, Dr Ivan Rungger.

An application was submitted in collaboration with QVEC to Royal Society Meetings: Quantum Computing in Materials and Molecular Sciences, proposed date if successful is September/October 2025. Applicants are Viv Kendon, Richard Catlow, John Buckeridge, Bruno Carmino and Alin Elena.

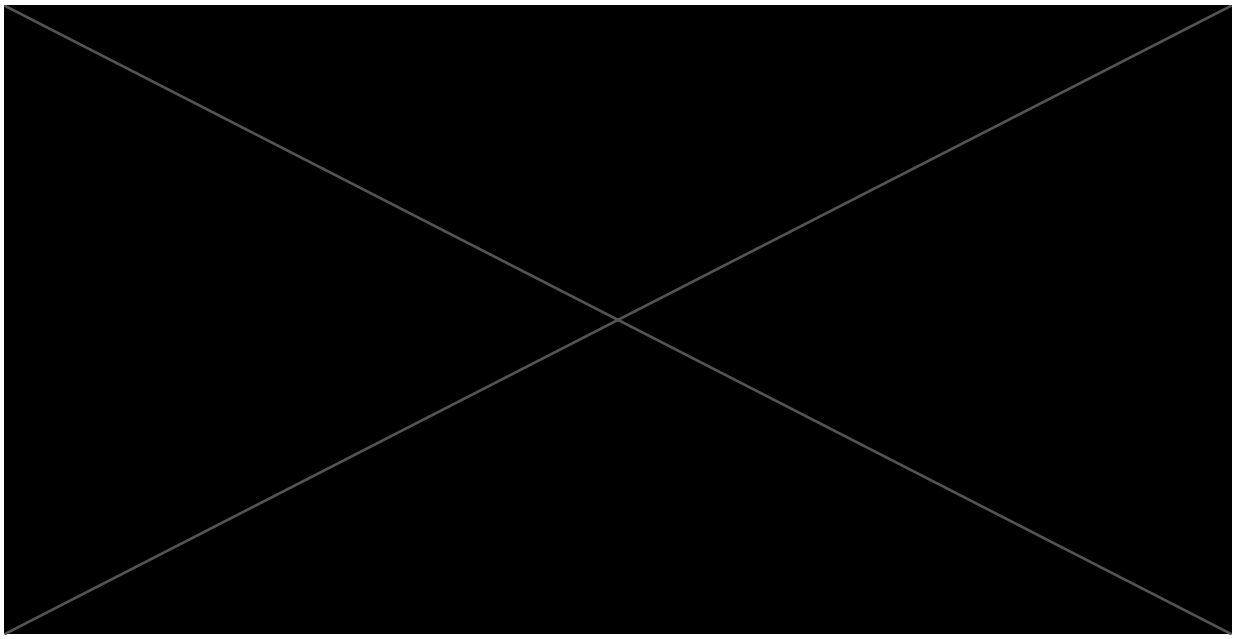
4. Resource Planning and Allocations 2023-24 and 2024-25

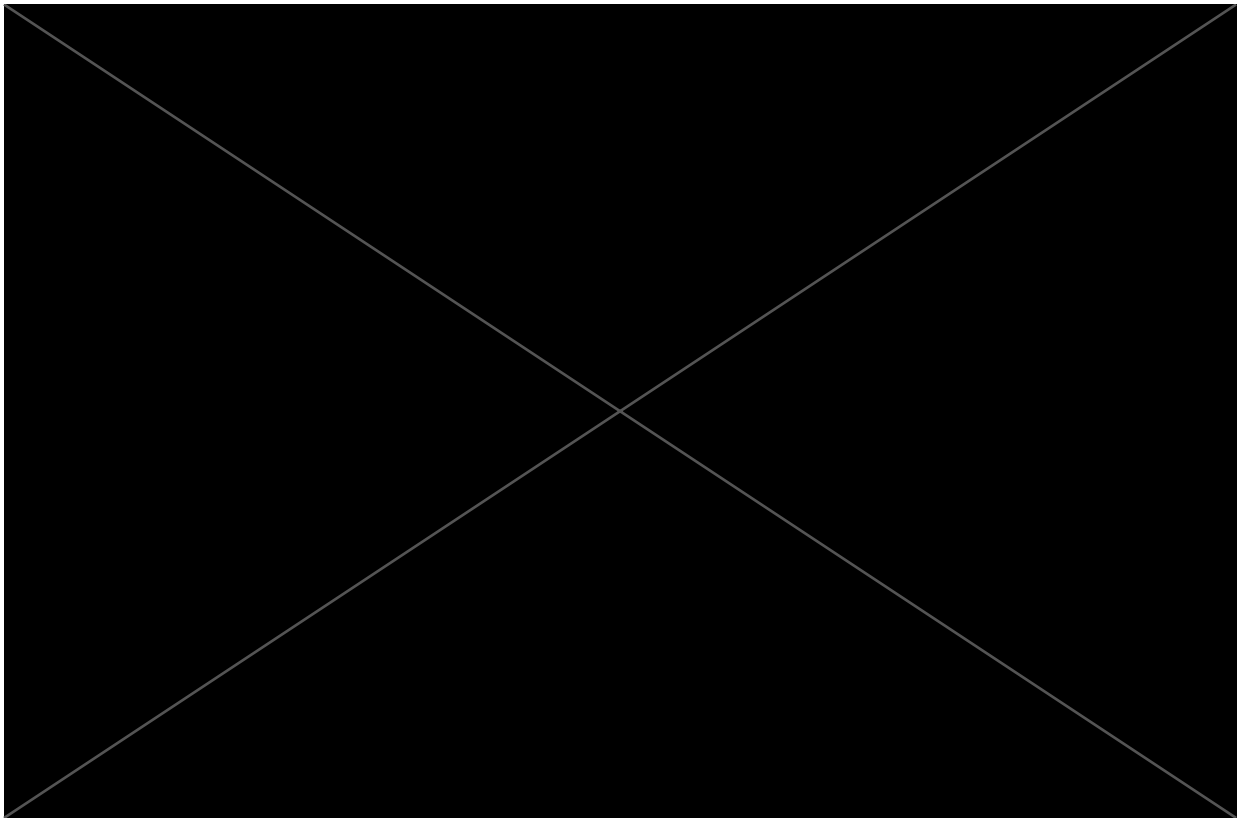
This section of the report outlines the financial details and resource planning for 2023-24 and looks ahead to 2024-25.

The costing for financial year 1 April 2023 to 31 March 2024 was calculated and agreed with EPSRC as follows:

	Staff (FTEs)	Pay (£K)	Overheads (£K)	Recurrent (£K)	Capital (£K)	Total (£K)
Support Functions	1.5	96.2	71.2	5.3	0	172.7
CCPs	12.6	804.9	595.6	44.1	0	1444.6
Consortia Support	5.7	340.6	252.1	19.9	0	612.6
Software Outlook	0	0	0	0	0	0
Grand Total	19.8	1241.8	918.9	69.3	0	2229.9

Table 1: Costing of CoSeC programme for financial year 2023-24.





5. Metrics 2023-24

This section of the report includes the CoSeC metrics for 2023-24.

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, i.e. 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.

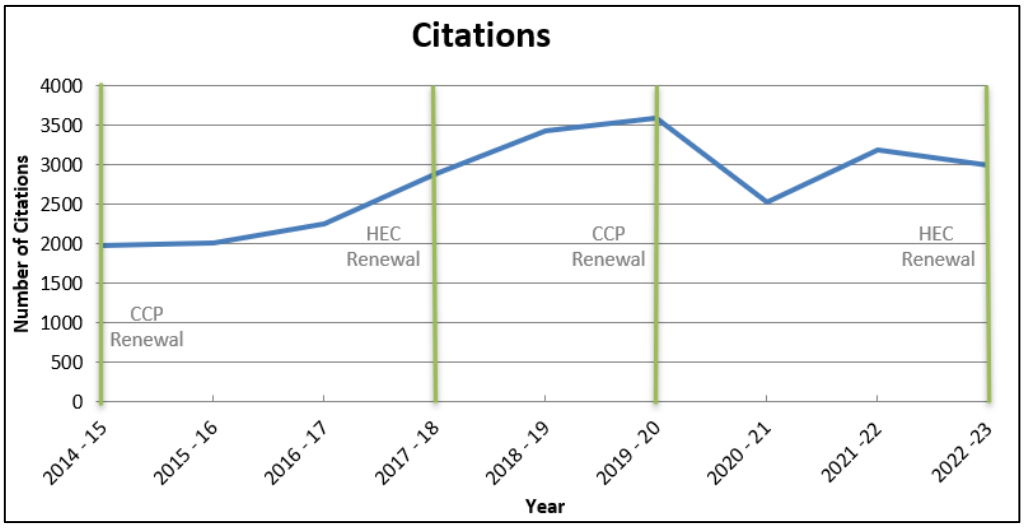
The trend in the metrics reflects the evolution of the programme brought about by the changes in communities supported at every renewal call. When considerable changes of the CoSeC communities occur, the metrics tend to decrease, and then recover as the new communities begin to grow their activities 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 a world-wide cost-free source-code academic license.

Metrics breakdown by area

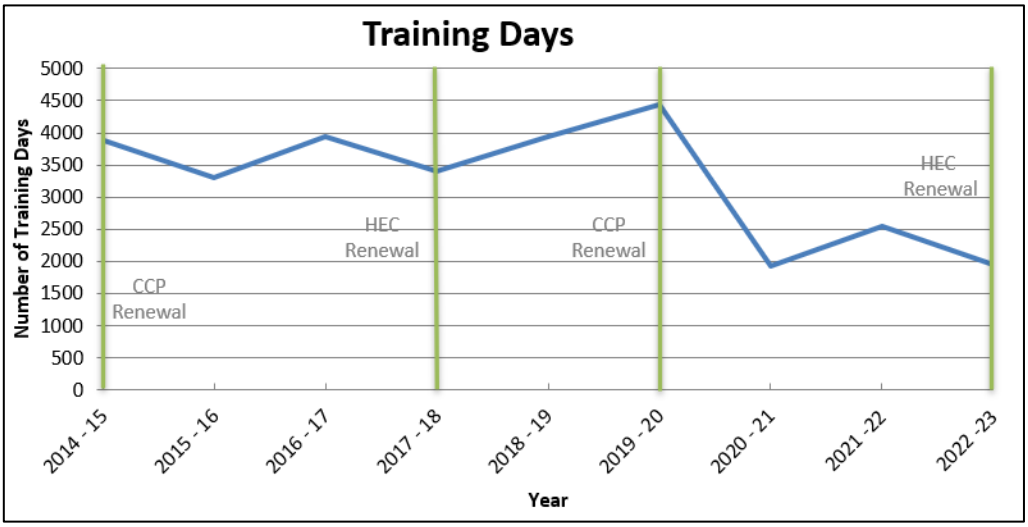
	FTEs Used	Publications	Presentations	Training Days	Citations
Materials Science					
CCP9	2.87	4	5	700	265
CCP-NC	1.24	2	1	208	57
UKCP (including CASTEP)	0.23	1	0	0	1755
MCC (including ChemShell, CRYSTAL)	2.12	11	5	490	692
Biological Science					
CCPBioSim	1.72	0	1	240	17
HECBioSim	0.80	0	3	0	0
Computational 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**

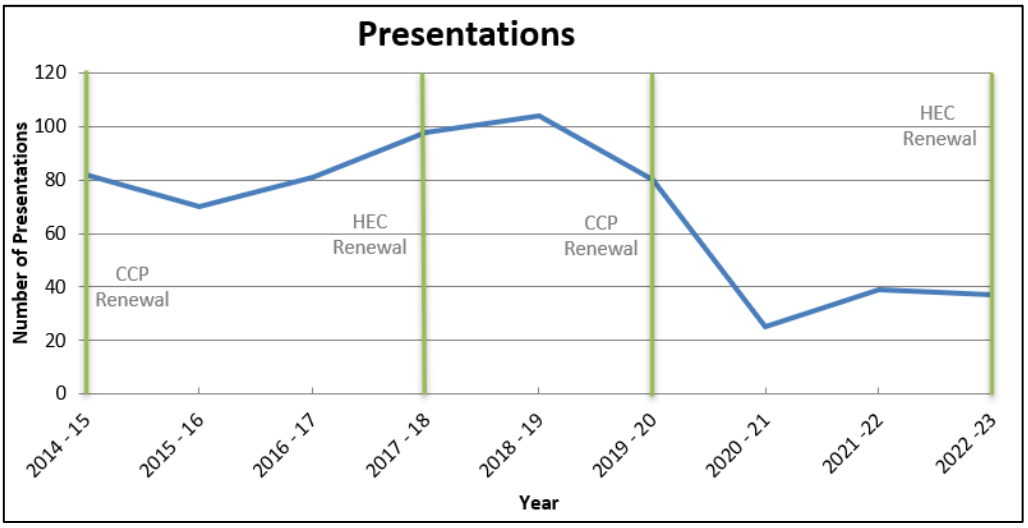
Table 3: Metrics breakdown for 2022-23 by scientific theme.



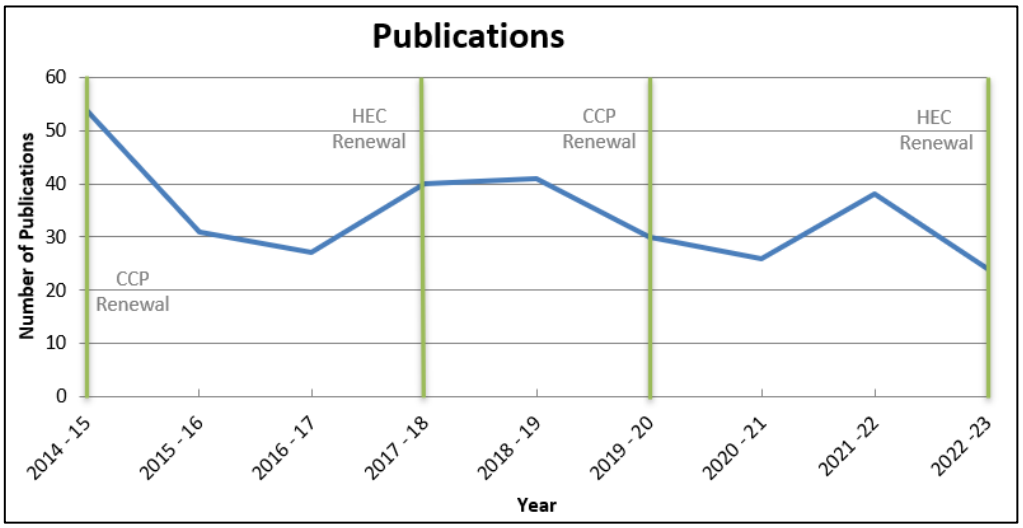
Graph 1: CoSeC Citations



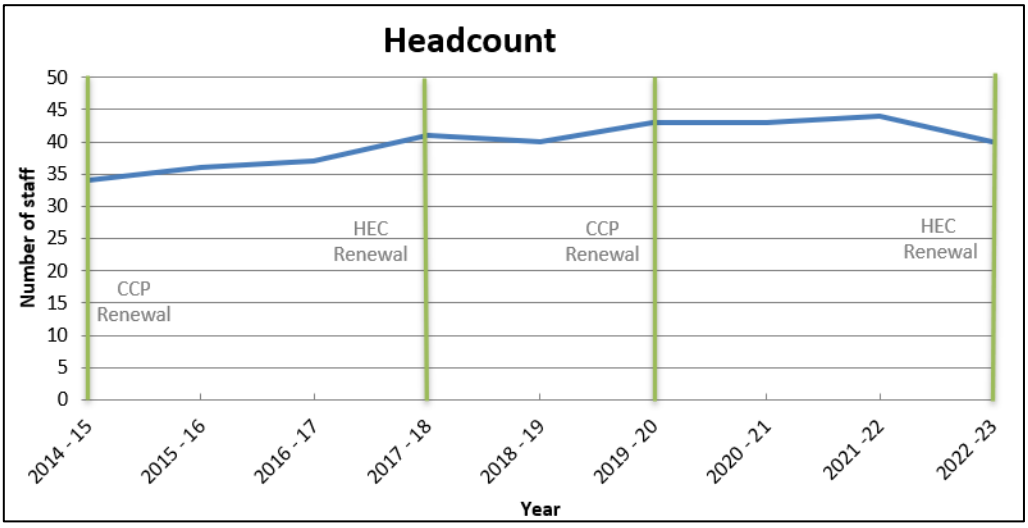
Graph 2: CoSeC Training Days



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 4: Community size by CCP/HEC.

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

Computational Science Centre for Research Communities

Financial Year 2023-2024 Annual Report

(*Covering the period 1 April 2023 – 31 March 2024*)

APPENDICES

Appendix 1 - Individual CCP/HEC Reports 2023-24

This appendix contains the full, individual summary reports for 2023-24 for the CoSeC supported CCPs and HECs.

Materials Science

CCP9

Wannier90: One of the major tasks within 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).
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 that was hosted at Daresbury laboratory in May 2023, with Jerome the local organizer. The code has been merged in the develop branch with the Wannier90 developer group at the February 2024 meeting at Paul Scherrer Institute, CH. Both developer meetings were co-organized by Jerome.

CRYSTAL: Barry was providing ongoing support for the CRYSTAL package, with the main development however now coming from an eCSE project. Application for GPUization of CRYSTAL code has been submitted to the eCSE-GPU.

ONETEP: Manuel has continued developing the ONETEP software package. The new stress functionality was presented at the ONETEP masterclass that took place on 22-24 August in RAL (https://onetep.org/news/onetep-masterclass-2023) and was meanwhile expanded with a robust algorithm for cell relaxation based on DIIS. The ONETEP UPF reader was extended to process not only norm-conserving but also PAW pseudopotentials, and the ability to extract spin-orbit-related information from the pseudopotentials is now merged into the main code.

QUESTAAL: Jerome has continued supporting and developing new features in the electronic software package QUESTAAL. New cRPA implementation merged into master; extension to multi-site interactions (cluster DMFT) started. A new TD-DFT like spin-wave maker has been implemented, applicable to GW as well as DFT and featuring a powerful plotting interface. BSE-susceptibilities ongoing. The QUESTAAL school took place at NREL in Denver, Colorado, with Jerome co-organizer and invited speaker as well as tutoring.

Collaborations in Materials Science: Jerome and Leon collaboration on calculating dielectric functions with Didier Sebilleau at Rennes University and Aditi Mandal at the Weizmann Institute, as well as ongoing collaborations with Sheffield/Leeds on magnetic properties of Mn2Au, and with Oxford on exchange interactions in 2D Fe5GeTe2. Manuel is continuing his collaboration with Juelich on the properties of a magnetic materials, which has resulted in there publications on respectively spin-

relaxation of Fe adatoms on MgO/Ag(100) [Phys. Rev. B **107**, 144417 (2023)], topological magnetism in $CrTe_2$ [Phys. Rev. B **108**, 094409 (2023)), and spin-dynamics of Mn_5Si_3 [APL Materials **11**, 081103 (2023)], and topological spin-waves in Mn_5Ge_3 [Nat. Commun. **14**, 7321 (2023)].

Manuel co-organised the WE Heraeus workshop – First-principles Green function formalisms: algorithms, method developments and applications to spinorbitronics and magneto-superconductivity, 4-7 September 2023, in Athens, Greece. The workshop was awarded €4,000 from the Psi-k Network and €23,000 from the WE Heraeus foundation.

The CCP9 Conference and Community Meeting was organized in Chester, in March 2024. The 3 day meeting was very well received, with over 100 participants, 13 invited and 28 contributed talks and 40 posters.

CCPNC

The CCP-NC successfully recruited to a joint CoSeC-PSDI position (started 04/09/2023) whose focus is re-developing our database of computed solid-state NMR quantities, prioritizing usability, and adherence to FAIR (Findable, Accessible, Interoperable and Reusable) principles. This collaboration is expected to foster productive interactions between PSDI and our scientific community. As PSDI's pathfinder project, we actively contribute to shaping their services and receive expert guidance for enhancing the CCP-NC database. Building on previous user consultations, we have improved both our own documentation and tutorials, as well as contributed to those of the CASTEP code. CoSeC staff (Kane Shenton) worked with the CCP-NC industrial-engagement post-doc during their placement in Johnson Matthey to develop functionality within our Soprano library to tackle defects in zeolites. This code is now being used internally in JM and an advanced tutorial has been added to the Soprano documentation on this subject. In addition, we have continued to contribute documentation and tutorials to a new CASTEP website.

CCP-NC have built on our developing connections to the muon spin resonance (μSR) community. We have adapted Galaxy platform's workflow management tools to provide support for three of CCP-NC's NMR post-processing tools, and plan to evaluate their usefulness for the user community. Our ongoing CCP-NC Online discussion meeting series has continued, with our most popular session so far being held in May 2023 on the subject of paramagnetic NMR calculations. CCP-NC hosted an online meeting in November 2023 on Organic Crystal Structure Prediction (CSP), with speakers from Cambridge Crystallographic Data Centre (CCDC). CCP-NC organised a joint meeting with CCP5 and CCP9, 'Taming Disorder in Solid Materials', in December 2023. The hybrid format worked well, with an approximately equal split between in-person attendees and the number online at any time. Although participation from CCP5 in particular was largely limited to the invited speakers, the feedback from participants was highly supportive of the programme format with constructive comments for improvements in future meetings.

UKCP

During the reporting period an additional 582 academic groups successfully applied for the free-of-charge source code licence. CASTEP 23.1 was released under the academic source code licence in May 2023 on the licences.stfc.ac.uk service. In August 2023 we made available the first public beta release of CASTEP for GPU. This feature compatible version of 23.1 allows use of server-grade GPU hardware to accelerate core functionality of CASTEP, reducing time to science. Full integration to a single code-

base has been rescheduled for academic release 25.1. In the meantime, a 24.1 feature-compatible GPU release is planned for summer 2024.

The continuous integration environment for CASTEP has been maintained and developed to include both build systems (GNUmake and cmake) and updated compiler configurations. Capabilities have been extended to test packaging for release and use of a static code analysis tool (produced by Peter Byrne at University of York as part of EPSRC grant EP/W030438/1). Our routine test process keeps the code-base for CASTEP in a sustainable state and minimises problems for developers and end-users. A direct benefit of these latest CI developments was our ability to release CASTEP 24.1 during March 2024, reducing the time between the commercial (outside of CoSeC support) and academic releases, compared to previous release cycles. Developer and community support was provided through code review (of "pull requests"), technical support for successful compilation of CASTEP and advising HPC centres on best practice for central installations of CASTEP that comply with licence terms. A user training workshop was held in York, September 2023 – see training section for details. The annual CASTEP core developers coding workshop (a.k.a. "Codefest") was held in person in March 2024. 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. Work has been carried out to design and prototype a CASTEP licensee database. This relates individual users to their research group licence. This is a core component of the planned academic CASTEP licensee query service that will allow HPC teams a secure and simple interface to check the licence status of users requesting access to centrally installed versions of CASTEP. The development and deployment of the web interface for this database will be continued through the remainder of 2024. John Trail has produced a report that details a novel extension to the generation of correlated-electron pseudopotentials to Density Functional Theory (DFT). This method naturally results in a description of the "removed" core electrons with higher accuracy than DFT. The report outlines paths to further research and directions for new methods that promise to improve the accuracy and transferability of pseudopotentials – a key method used in many electronic structure codes, including CASTEP.

MCC

Ab initio DFT: CRYSTAL23 is rebuilt and running on the upgraded ARCHER2 software environment, and issues reported by users are being addressed as they occur. A blueprint for interoperability of CRYSTAL and CP2K restart data is complete and the implementation phase is underway. Relevant, unsymmetrised, data, such as the basis set and density matrix, can be saved from CRYSTAL in an appropriate format.

Classical and ML forcefields: DL_FIELD has been extended to process CHARMM format files, extending DL_FIELD's capability to access third party force field webservers such as OPLS's LigParGen and CHARMM's MATCH. Work to enable the Hill-Sauer zeolite forcefield in DL_FIELD is complete and version 4.10 has been released. A DL_POLY hackathon and training event has been held and an MCC user community workshop is being planned. ML interatomic potentials have been assessed for benchmarking studies of the structure and dynamics of MOFs, comparing various ML approaches vs classical forcefields and DFTcalculations.

Multiscale methods: Tcl-ChemShell and Py-ChemShell have been rebuilt and tested following the upgrade to ARCHER2's software environment. The embedded cluster model for covalent materials in ChemShell has been benchmarked using the hybrid MPI/Open MPQM code LSDalton, in comparison

to NWChem, for energies, gradients and polarisabilities, and optimal compilation and runtime settings have been identified for both codes on ARCHER2. An improved transition state search method (STQN) has been implemented in the DL-FIND geometry optimisation library. 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.

Biological Science

CCPBioSim

Work continues on CodeEntropy. The purpose of the software is to calculate entropy from molecular dynamics trajectory data using the multiscale cell correlation method. Previously, the first release was made after work combining separate code for solutes and water into one program. From June, we have been working on the next stage of improvements. The definition of axis for the residue level units has been changed from a custom system of selecting three atoms to a method using the bonds between residues or principal axes for isolated residues. This will make the code more flexible in its ability to handle different types of molecules. Further work on refactoring the code continues. This should make the code easier to maintain and paves the way for future work on performance optimisation. We are adding functionality to calculate the conformational entropy at a residue level to work with systems which could change secondary structure such as intrinsically disordered proteins and extending the calculation of orientational entropy to molecules other than water.

The Docking Workflow project has finished. There are a set of Jupyter Notebooks which guide students through docking a set of ligands to multiple poses of a protein and analysing the results. Designed for students starting to learn about medicinal chemistry research these notebooks have been packaged into a virtual machine which was used at the September Training Week and then made available afterwards for anyone who is interested.

The 5th Manchester Multiscale Conference took place 3-5 April 2023. There were 82 in person participants and 14 online attendees. There were 8 invited speakers: Björn Baumeier (TU Eindhoven), Paola Carbone (University of Manchester), Cecilia Clementi (FU Berlin), Rosana Collepardo (University of Cambridge), Halim Kusumaatmaja (Durham University), Laura Orellana (Karolinska Institute), Modesto Orozco (IRB Barcelona), and Matteo Salvalaglio (University College London).

The CCPBioSim Annual Conference in July was also well attended with 100 people in person and 20 online. The theme this year was biomolecular simulations for a better world.

The online Industry Talks continue to be a great series. In this reporting period we have had talks by Alexander D. MacKerell of SilcsBio LLC, Antonija Kuzmanic from Schrodinger, Huafeng Xu from Atommap, Peter Kenney, David Wright from KuanoAI, David Hardy from the NAMD development team, and Brian Bender from SoseiHepatares. The attendance is 50 to 100 people at each seminar and they actively participate with lots of questions for the speakers.

HECBioSim

In the current reporting period considerable effort has been spent on supporting users with HPC on ARCHER2, JADE2 and Bede. In this reporting period, there has been an increase in projects that have users from non-traditional HPC backgrounds or users of a novice experience level, such as collaborations with experimental groups. This has presented as a significant increase in users asking for help with software packages outside of the consortium core supported codes and also in users not

obtaining desired performance results. This challenge has been met by the provision of upskilling and advice as well as targeted profiling/benchmarking and debugging of software issues, resulting in upskilling and users obtaining scientific results more inline with expectations.

Software maintenance across the HPC machines, there was an issue on Bede where some software packages either disappeared or were corrupted. There was an unplanned power outage around the time this emerged, so although the cause is currently unknown it is likely related. A number of software packages and libraries had to be rebuilt and then retested for correctness and performance since they were complete rebuilds and some minor system packages had been upgraded since first builds. On JADE2 there are a number of issues in the software build environment that are preventing some software packages from being built, mainly this is affecting AMBER22 and the latest OpenMM packages. This has been isolated to issues with the CUDA driver and CUDA libs being out of sync or with partial compatibility, we are coordinating with Hartree systems team in how best to resolve this upon which the packages in question will be made available. There was also a CVE in the openmpi 4.0.5 on JADE2 and this required moving the version forward to 4.1.5, meaning all software packages maintained by HECBioSim had to be tested for correctness and performance and where issues occurred, the package rebuilt. HECBioSim access to JADE2 ceased in March 2024, which has placed a burden upon technical support in assisting the Hartree Centre with a controlled reduction of data storage and user accounts. This placed a considerable time burden to coordinate the organised withdrawal of our community from a service that is continuing to operate beyond its end of life, albeit with a reduction in communities that have access.

Work has been progressing on modernising the HECBioSim website from the existing end-of-life Joomla 3 to the new Joomla 5framework. There are a number of advanced components of the website, such as the HPC resource calculator that have presented more of an issue than expected in bringing forward into the new framework. However work is progressing and it is anticipated that the website will be delivered slightly behind schedule. The new website will offer many more advanced features, such as a more advanced and integrated HPC resource calculator, such that it can be used whilst applying for resources. The applications will be tied to accounts so that academics can get a report for use with REF, also the panel will be able to get information in the correct format via the website rather than relying on spreadsheets and dropbox which has become unwieldy to keep track of as the number of machines increases.

Work to introduce features to Longbow have been paused in the interim whilst we take the decision on the future of the package. There are a number of options available that we are considering, such as retiring Longbow and support other software packages (Crossflow, AiiDA etc) by migrating some of the advanced features from Longbow to those packages.

Benchmarking of HPC resources has continued as new packages have been released. There are new features in AMBER22 for multi-GPU simulation, which we will investigate but build issues have held this work back. New versions of GROMACS and NAMD have been tested on all machines and have shown improvements in performance. The ExCALIBUR grant for ExaBioSim has been funded so we are working on integrating our benchmarks with the new ones that will emerge from that project to greatly enhance the benchmarking data that we have available to cover vastly more software and physics within them. The ground work has been laid for the openmm benchmarks by converting the system to the correct format but further testing needs to be done to ensure these are truly the same as with the other packages. The multi-GPU work will now be deferred to the ExaBioSim consortium

since they will also be looking at this across a much deeper range of codes and physics. We are jointly developing an automated benchmarking suite of tools called hpcbench . We have also been evaluating using DiRAC as a consortium supported HPC machine, which has involved benchmarking and evaluating the software stacks available on the various machines within DiRAC.

We have been working on re-establishing the software development activities for HECBioSim. This has been mainly focused around starting up the project around DeepDriveMD which has been delayed due to recruitment of the post-doc based at Oxford. Scoping work has also concluded on a second software project to bring Edina Rosta's string based enhanced sampling code to a generalised and HPC efficient status. Work on both of these will start in earnest in the 24/25 reporting year.

Computational Engineering

UK-COMES

Preparations for a new release of DL_MESO are underway, which is expected in Q2 2024. As well as completion of a new graphical user interface based on Python and Qt to enable users to get started more easily with DL_MESO simulations, new features have been added to the DPD and LBE codes. A Large Eddy Simulation (LES) model has been added to the LBE code to enable higher Reynolds number flows with turbulence to be modelled, as well as the Cross model to provide more realistic rheology for polymer melts and dispersions. A generalised many-body DPD model has been included in the DPD code to enable multiple-component simulations with larger density contrasts, including solid-liquid transitions, and efficiency improvements have been made in implementing exclusions of short-ranged interactions between bonded particles for more accurate modelling of smaller scale (but still mesoscopic) molecular systems.

CCP-WSI+

During this reporting period each work package of the CoSeC support for the community has progressed in a number of ways, as detailed below. The overarching Software Strategy for the community has been updated and continues to drive the overall work delivered by CoSeC's support.

WP1: In software terms, the work for this period has been driven by the overarching goal defined in the CCP-WSI+ software strategy around the creation of a multi-physics simulation environment for floating offshore wind turbine (FOWT) modelling, the ongoing CCP-WSI+ community blind test problem of focused wave interactions with a submerged flexible membrane has also been considered. The FOWT problem demands a significant amount of physical modelling capability and realistically can only be handled using a partitioned coupled approach as adopted by CoSeC's open-source Parallel Partitioned Multi-physics Simulation Framework (ParaSiF - https://github.com/ParaSiF/ParaSiF).

Currently the focus for ParaSiF is robust and scalable Fluid Structure Interaction as this captures the basic required by the FOWT problem and provides the majority of the solution for the flexible membrane case. A key focus during this reporting period has been around the structural mechanics solution within ParaSiF developed around the open-source Finite Element code FEniCSx. The current solver is based on an old version of FEniCS, however this is now deprecated, with only the FEniCSx version supported. The ParaSiF structural element is undergoing conversion from one codebase to the other, however this has highlighted a number of areas where the new code is fundamentally different to the old, with some necessary capabilities missing and others changed. The move to the latest code is imperative to allow the capabilities in ParaSiF to evolve to a point where problems like a think

flexible membrane can be tackled easily, therefore a significant amount of effort has been spent during this period on this.

CoSeC is working directly with the main development team of FEniCSx at Cambridge University, with some new capabilities being added fundamentally and aspects of the ParaSiF solver being redesigned. This work is ongoing but significant progress has been made. Work has also continued on the OpenFOAM elements of ParaSiF, with the latest version of the Multiscale Universal Interface (MUI) code coupling library developed by CoSeC fully integrated into its custom interFSIFoam and pimpleFSIFoam solvers.

The MUI library has also seen a major new release during this period, version 2.0 formally integrates a number of significant developments that can be directly attributed to the feedback and guidance received from the WSI community. During this reporting period, a process has been agreed with ESI to enable the direct inclusion of MUI into future releases of OpenFOAM. CoSeC is currently engaging with this to integrate its MUI/OpenFOAM deployment.

WP2: During this reporting period this WP has focused on producing test cases and coupled examples, including the flexible membrane test case from the blind test series, where an example test case using the PreCICE Coupling library to couple OpenFOAM interFOAM with Solids4Foam has been developed to match the experimental set-up of the flexible membrane. In addition, the overset capabilities in OpenFOAM was tested with several example cases. The main objective is to couple the overset mesh capabilities of OpenFOAM with an external solid mechanics solver using the PreCICE coupling library. Several smaller test cases were developed to verify the capability of the coupled software system with established results found in the literature, with results presented at international conferences.

Work to complete an integrated dynamic domain decomposition library have also continued during this period with results being fed back into the CCP-WSI repository.

WP3: The CCP-WSI catalogue remains the main focus of WP3 and is going through a change as the underlying platform that the catalogue uses is no longer supported. Work has concentrated this reporting period on development of the software resource type using the current framework whilst simultaneously investigating new platforms to replace it. There are many cataloguing needs across STFC (eg ePubs, eData and in the Technology departments as well as in CoSeC) and we hope to work with our colleagues to agree on a single platform going forward. This would mean that resource can be shared and more achieved overall.

This WP continues to support both CCP-WSI and HEC-WSI with their websites providing training and troubleshooting with content additions as well as high level website support. Work has been done, particularly, around data protection and this is a positive step going forward to meet the HEC's reporting needs.

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.

CCP Turbulence

The stable version 2.0 of 2DECOMP&FFT (https://github.com/2decomp-fft/2decomp-fft/tree/main) has been released together with a publication on the Journal of Open Source Software JOSS (https://joss.theoj.org/papers/10.21105/joss.05813). The submission was underpinned with the creation of a complete documentation (https://2decomp-fft.github.io/) together with a large comprehensive testing of the library on both Archer2 for CPU (https://2decomp-fft.github.io/pages/benchmarks_archer2.html) and cirrus for the GPU implementation (https://2decomp-fft.github.io/pages/benchmarks_cirrus.html).

Results have shown that the library is keeping the good original performances for the CPU part, and they show also relatively good performances with a good speed-up (in the region of 2-5) for the GPU acceleration. The main result is, however, the better performances for GPU acceleration given by the usage of a 1D-slab decomposition over the 2D-pencil decomposition.

Work to include OpenMP GPU offloading for 2DECOMP&FFT has also carried out. A multi-GPU version using NVHPC has been tested and work is going to adapt the work for other compilers starting from GNU.

The new version of the library has also been at the base of the new stable release of Xcompact3d V5.0 (https://github.com/xcompact3d/Incompact3d/releases/tag/v5.0), where 2DECOMP&FFT is a mandatory external library. The new release of the solver has also Magneto Hydro Dynamics (MHD) capabilities that have been tested with a 3 different test cases. A proposal to the ARCHER2 Pioneer call titled "Particle clustering in homogeneous and non-homogeneous turbulence with and without magnetohydrodynamic effects" has been submitted and based on the code developments recently done by Jian Fang for Xcompact3D. The proposal had been successful and 0.5M CU of computing time had been awarded. Work on OPS has also restarted with regular catchups. The CI framework has been

fixed and an update of the CMake build system is on-going. This work is to support a new release of the library. Work has also been done on the code ASTR to a chemistry reaction module and low-density flow module, related to combustion and rarefied gas dynamics respectively. This work has been presented in several meetings and to the Royal Aeronautical Society.

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 19 July 2023 we released SIRF 3.5. In this release we replaced the temporary Python implementation of the acquisition and image data algebra used in previous releases with a proper C++ one interfaced into Python by SIRF's standard simple wrapping, which eliminated creation of multiple

temporary copies of data. On MR side, SIRF 3.5 allows the use of radial, golden angle, spiral and RPE trajectories of raw data acquisition and allows the user to modify the reconstructed k-space dimensions, which enables e.g. retrospective motion resolved or time-resolved reconstructions, or combinations of such dimensions. We also added Gadgetron gadgets that allow for k-space filtering, coil compression and partial Fourier reconstruction. On PET/SPECT side, we added interfaces to various STIR functions,which affords the user more control of the reconstruction.

Another major development was the creation of a new WordPress powered website for our project, which took several months, new website becoming live on 27 July 2023. Also, the phantom data to investigate head motion correction methods for PET/MR, acquired in Leipzig, was uploaded to Zenodo.

On 15 Feb 2024 we released SIRF 3.6. In this release we added extra members to ScatterEstimation class to set behaviour of OSEM used during scatter estimation, added test for scatter simulation and estimation, fixed randoms' estimation and ensured compatibility with STIR 6.0. On MR side, we improved handling of "irregular" ISMRMRD acquisitions by providing IgnoreMask object that allows the user to specify which kind of acquisitions is to be ignored. We also improved our Python interfaces to STIR, Gadgetron and Nifti data containers, having significantly reduced copying data between Python and C++ code, and fixing handling of complex images by our Nifti registration interface.

Quantum Computing

CCP-QC

Scientific Applications of Quantum Computing: Materials, Chemistry and Biology, September 22, 2023 organised at LSE Bankside London was an important opportunity for a number of companies and academic teams to offer their experimental and commercial developments in the quantum computing for work in different areas of science and engineering. The meeting brought together representatives of the industrial and academic communities active in the world of quantum computing and computational scientists in materials science and related areas of physics, chemistry, engineering and life science. The aim was to highlight the new opportunities and explore what quantum computing can offer us now and in the near future. For example, can quantum computing tackle our current computational problems that we address with "conventional" supercomputers and at what cost, what alternative approaches the quantum computing can offer us opening new avenues, perhaps, allowing us to approach currently unfeasible tasks or impossible challenges? Conferences was co-organised by various CCPs with participation from, MCC, CCP5, BioSim, HecBiosim, UKCP, CCP9 and CCP-QC in addition to industrial participants, from startups as Riverlane and Seeqc to well established companies as Johnson Matthey. AE was part of the organising committee.

https://web.cvent.com/event/d87cb285-da12-476c-83c0-9bbda9b765ba/summary

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 2023-24

This appendix contains updates on code developments during 2023-24.

Materials Science

CCP9	Code Development	Comments
CRYSTAL	Planning for future release	ongoing
ONETEP	• stress-tensor of the unit-cell parameters • read pseudopotentials in UPF file format • spin-orbit-related information from the pseudopotentials • check-pointing functionality	• complete • complete • complete • planning
QUESTAAL	• new cRPA implementation • extension to multi-site interactions • spin-dependent BSE-susceptibilities	• complete • ongoing • ongoing
W90	• type definition and classification • error handling • library interface • documentation/testing	• complete • complete • complete • ongoing

CCPNC	Code Development	Comments
Soprano	• Expanded command-line interface functionality – available on bleeding edge version with documentation. • New long-form tutorial on defects in zeolites. • Major Euler angle refactor, including generation of comprehensive test suite	• Complete • Complete • Ongoing
MagresView 2.0	• Euler angle visualisation support various eigenvalue ordering conventions • Expanded support for visualising Euler angles of dipolar tensors • User evaluation of added Euler angle visualisation functionality	• Complete • Complete • Ongoing
orgdisord (formerly: SODORG renewal)	• Migrate code base to permanent home under the CCP-NC GitHub organisation • Bug fixes to handling of certain Z' ≠ 1 cases and the specification of disorder by inputting two ordered structures • Refactoring to allow for better flexibility in defining disorder	• Complete • Complete • Complete
CCP-NC Magres database	• Develop implementation roadmap for CCP-NC database with CCP-NC and PSDI • Maintenance and further development of CCP-NC database – adding support for more complex search queries • Replace existing API for the CCP-NC database • Rebuild CCP-NC database software stack, replacing AngularJS	• Complete • Ongoing • Ongoing • Ongoing

MCC	Code Development	Comments
ChemShell	• Rebuild of Py-ChemShell and Tcl-ChemShell for the upgraded ARCHER2 software environment. • Performance improvements for QM/MM calculations using LSDalton and NWChem on ARCHER2	• Complete • Complete
DL-FIND	STQN transition state search approach implemented in DL-FIND	Complete
CRYSTAL	Rebuild of CRYSTAL23 for the upgraded ARCHER2 software environment.	Complete
DL_FIELD	• Extension to process CHARMM format files • Inclusion of Zeolite Hill-Sauer FF with auto identification of atom types. • Released version 4.10	• Complete • Complete • Complete
Janus-core	Development started for easy access to ML forcefield and various modelling techniques. (https://github.com/stfc/janus-core)	Complete

Biological Science

CCPBioSim	Code Development	Comments
CodeEntropy	• Improving the axis definitions • Restructuring the code to remove duplicated functions and make the flow clear • Refactoring to use the MDAnalysis classes and library • Adding the calculation of conformational entropy at the residue level • Adding the calculation of orientational entropy for molecules other than water	• Complete • Complete • Complete • Complete • Ongoing

HECBioSim	Code Development	Comment
hpcbench	First release of the automated benchmarking suite developed as a joint collaboration with hecbiosim and exabiosim.	

Computational Engineering

UK-COMES	Code Development	Comment
DL_MESO	• New Python/Qt graphical user interface • Generalised many-body DPD • Large Eddy Simulation (LES) model in DL_MESO_LBE	• Complete • Complete • Complete

CCP-WSI+	Code Development	Comments
Research Object Catalogue	Platform 1. Investigating new underling platform options Admin 1. First (soft) Release 2. Software resource type added for next release Projects & Test Cases 1. First (soft) Release 2. Implement changes resulting from feedback Software 1. Requirements gathering Publications 1. Requirements gathering	1. Complete 1. Complete 2. Complete 1. Complete 2. In progress 1. In progress 1. On-hold due to new framework
Parallel Partitioned Multiphysics Framework (ParaSiF)	1. Release as open source on GitHub 2. Port and compiled on ARCHER2/SCARF 3. Integrate MUI into latest ESI OpenFOAM 4. Release MUI integration publicly 5. Redesign *interFSIFoam* solver from ParaSiF for latest ESI OpenFOAM release 6. Update FEniCS structural solver to FEniCSx 7. Add additional structural modelling capability to structural solver for thin membrane problems 8. Integrate harmonised CCP-WSI *interFoam* solver into redesigned *interFSIFoam* solver and release via CCP-WSI repository.	1. Complete 2. Complete 3. Complete 4. In-progress 5. Complete 6. In-progress 7. In-progress In-progress
Multiscale Universal Interface (MUI) code coupling library	1. Maintain and support library for WSI community 2. Develop parallel performance of library for use on highly parallel architectures like ARCHER2 3. Integrate the library generally into ESI OpenFOAM and release directly through openfoam.com	1. Ongoing 2. Complete 3. In-progress 4. Complete 5. Complete 6. Complete

	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	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 CCP-WSI 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
CHAPSim2.0	Implementing a pre-/post-processing procedure to handle staggered grid in the Poisson solver	Complete
CHAPSim2.0	Implementing a sine/cosine Transformation in the code for various boundary conditions in the Poisson solver	Complete
2decomp&fft lib	Implementing the 3-D sine/cosine Transformation (based on FFTW3) to the library of 2decomp&fft	Complete
CHAPSim2.0	Added Paraview compatible format 'xdml' for data output including raw data and space/time averaged data	Complete
CHAPSim2.0	Carrying out performance of CHAPSim2 in Archer2	Complete
CHAPSim2.0	Implementing the cylindrical coordinates to CHAPSim2 for pipe or annular flow simulation	on-going
CHAPSim2.0	Support the development of immersed boundary conditions for CHAPSim2.	on-going
CHAPSim2.0	Support the development of multiphase flow simulation in CHAPSim2.	on-going

UKTC	Code Development	Comment
	No code development activities	

CCP Turbulence	Code Development	Comment
2DECOMP&FFT	Release of version 2.0	Complete
Xcompact3d	• Release of version 5.0 of the code with 2DECOMP&FFT and MHD • Particle tracking module for simulation of multi-phase flow.	• In beta version • To be merged
ASTR	• Chemistry reaction module for simulation of reacting flow, e.g. combustion. • Low-density module of simulation of rarefied gas dynamics.	• Complete • Complete

Tomographic Imaging

CCPi	Code Development	Comments
CIL	Optimisations of SIRT algorithm, L2NormSquared and MixedL21Norm functions	complete
CIL	Development of the warm start functionality for the regularisation function Total Variation, leading to a considerable acceleration of the code.	complete
CIL-GUI	0.5.0 to 0.5.3 releases with new functionality and bugfixes.	

CCPSyneRBI	Code Development	Comments
SIRF	• Replace Python implementation of DataContainer methods with simple Python wraps of their C++ implementation. • Provide C++ tools for accessing the examples data. • Allow user to set radial, golden angle, spiral and RPE trajectories. • Add Gadgetron gadgets that allow for k-space filtering, coil compression and partial fourier reconstruction. • Add SIRF interfaces to more STIR functions. • Add Time-of-Flight support for PET data reconstruction. • Add extra members to ScatterEstimation to set behaviour of OSEM used during scatter estimation • Add missing set/get methods for OSSPS step-size relaxation • Improve handling of "irregular" ISMRMRD acquisitions by providing IgnoreMask object that allows the user to specify which kind of acquisitions is to be ignored.	• Complete • Complete • Complete • Complete • Ongoing • Complete • Complete • Complete • Complete

Appendix 4 – Training and Outreach 2023-24

This appendix contains updates on training and outreach activities during 2023-24.

Materials Science

CCP9

- Barry gave 2 lectures at the CCP5 summer school advanced course for First Principles simulation, 25-27 July in Durham:
    - "Quantum chemical methods"
    - "The CRYSTAL code."
- Manuel gave three presentations on "Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3" at
    - Theoretical and Experimental Magnetism Meeting, 21 June 2023 at The Cosener's House, Abingdon
    - Condensed Matter and Quantum Materials Magnetism conference, 29 June 2023 at the University of Birmingham
    - (Invited) IoP Magnetism conference, 3 April 2023 at the University of Manchester
    - CCP9 Conference and Community Meeting, 19-22 March 2024, Chester.
- Manuel presented a poster entitled "Complex magnetism and spin dynamics of Mn5Si3 and Mn5Ge3" at the IOP Magnetism 2024, 25-26 March 2024, Loughborough, and was awarded a poster prize.
- Jerome gave an invited talk entitled "Quasi-particle self-consistent GW in QUESTAAL" at the First-principles Green function formalisms: algorithms, method developments and applications to spinorbitronics and magneto-superconductivity workshop, 4-7 September 2023, in Athens, Greece.
- Jerome gave 2 talks at the "5th Questaal school" that took place 11-14 March 2024 at National Renewable Energy Labs, Golden CO:
    - "Introduction to the full-potential code, lmf"
    - "Spin-waves with QUESTAAL."
- Leon presented a poster entitled "Complex magnetism in Gd-intermetallics" at the First-principles Green function formalisms: algorithms, method developments and applications to spinorbitronics and magneto-superconductivity workshop, 4-7 September 2023, in Athens, Greece.
- Barry gave a talk on 15 May at the Wannier90 developers meeting titled 'Wannier90 library developments'. This is work done with Jerome and Leon as part of the CCP9 CoSeC support.

CCPNC

Our ongoing discussion meeting series, CCP-NC Online, has had five meetings to date, with the most popular (109 participants with 58% participation from academic institutions and companies from outside the UK) of these occurring during this reporting period, partly due to expanded advertising to international mailing lists. We continue to engage with new and existing community members through feedback forms after the meetings to gain valuable insights into their interests. This user feedback is used to guide in prioritising our software and science support efforts.

CoSeC staff are normally involved with annual CASTEP training workshops. However, the workshop this year in York was intentionally a smaller scale event than usual and so we did not send support staff to help with the tutorials and lectures directly.

UKCP

The annual CASTEP teaching workshop was held in York, September 2023. Dominik Jochym provided support during 2 of the 5 days of the workshop, advising participants during tutorial sessions and technical support to convert and deploy web-based training material. The full workshop ran 18-22 September 2023 for 25 participants.

MCC

- The 2023 MCC conference was hosted at Daresbury Laboratory, 28-30 June. Local organisers Georgia Lomas, Alin Elena and Tom Keal worked with Scott Woodley and Richard Catlow to arrange the 3 day event, which included talks from MCC members and external speakers grouped around the nine MCC themes, a poster session, and conference barbecue dinner.Over 80 people attended the event.
- Tom Keal gave his inaugural lecture as a visiting professor at UCL Chemistry on 27th April on "Scaling up computational chemistry: from small molecules to complex systems." Kakali Sen also presented on "Modelling enzyme reactivity with QM/MM simulations" along with speakers from St Andrews, UCL and QMUL. Approx. 50 people attended the symposium.
- You Lu led a software spotlight training seminar on ChemShell on 25th April.
- Alin Elena organised the Machine Learning for Atomistic Modelling Autumn School 2023, held on 18-20 September at Daresbury. 31 students attended the event.
- MCC co-sponsored a workshop on Scientific Applications of Quantum Computing on 22 September. Alin Elena was one of the organisers and Tom Keal gave a talk at the event.

Biological Science

CCPBioSim

There was an OpenMM workshop with 30 in person and 15 online participants at Leeds on 12 July 2023. The CCPBioSim Training week was also in Leeds, 25 – 29 September 2023. This week had 6 different workshops – Python, BioSimSpace for Free Energy Calculations, Docking, Introduction to Amber, CodeEntropy, and Open Force Fields. There were 180 registered participants (30 in person and 150 online).

HECBioSim

HECBioSim delivered its first training course jointly with the CCPBioSim on the building and running of complex biomolecular simulation workflows and using them on HPC systems. In the case of this workshop it was demonstrated how workflows could be built with CrossFlow workflow tools and then run them on ARCHER2.

HECBioSim also supported the following workshops with HPC and software support for their workshops:

A joint EBI-CCPBioSim workshop on "structural bioinformatics resources and tools for molecular dynamics simulations" – held on 19th - 22nd September

The CCPBioSim training week – held on 25th - 29th of September

Computational Engineering

UK-COMES

Michael Seaton contributed to the CCP5 Summer School in July 2023 held at Durham University, providing seminar talks on DPD and practical exercises for both DPD and LBE using DL_MESO to 10 students. He contributed a talk to the CoSeC Annual Conference on Day Zero of Computing Insight UK 2023 (held in Manchester on 6-8 December), "Thermodynamically Consistent Multi-Phase DPD".

He is contributing further training materials on DPD and LBE to the DL_Software Digital Guide (https://dl-sdg.github.io/).

Jianping Meng had a conference talk accepted for the 2023 International Joint Conference on Civil and Marine Engineering held in Dalian, China on 3-6 November – Simulation of the floating objects with Lattice Boltzmann Method – based on HiLeMMS work.

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.

CCP Turbulence

A two-day training event at The Cosener's House has been delivered covering the OPS library and the openSBLI solver. The training involved 31 participants with lectures and practical exercises delivers by expert in the fields of computer science (OPS) and supersonic aerodynamics (openSBLI) coming from University of Marwick, University of Southampton, Japan Aerospace Exploration Agency (JASA) and STFC.

A second training related to code_saturne and HPC has been organised together with CINECA and with the support of CECAM. The course has been attended by 20 persons with a mix of students (both at master and PhD level), research associates and professionals.

Tomographic Imaging

CCPi

During the reporting period Edoardo Pasca presented CIL at the Applied Inverse Problems 2023 conference (Goettingen, Germany) September 2023

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

- CIL-GUI training with EPAC on 8 June 2023
- 8th annual CINEMAX Summer School on 3D imaging, at Fuglsang Manor 21-25 August 2023
- 1 day training session on CIL at the Rosalind Franklin Institute, 5 trainees on 1st August 2023
- 1 training day on CIL at the Institute of Radiation Physics of the University of Goettingen, 6 September 2023

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

CCPSyneRBI

On 13-14 Nov 2023, we held our first Hackathon on the Emission Tomography Standardization Initiative (ETSI, established end 2021) that is working towards a standard for PET listmode and associated data called PETSIRD.

On 12-14 Jan 2024 we held another Hackathon where we worked on topics related to our PET Rapid Image Reconstruction Challenge.

Quantum Computing

CCP-QC

Scientific Applications of Quantum Computing: Materials, Chemistry and Biology, September 22, 2023, see above for details. A perspective paper including all invited speakers is in preparation.