Financial Year 2021-2022 Annual Report

(*Covering the period 1 April 2021 – 31 March 2022*)

Report Submitted June 2022

Contents

Executive Summary

The reporting period from April 2021 to March 2022 has seen further evolution of the CoSeC programme to group support effort by scientific field rather than by individual CCP or HEC while maintaining an approach that delivers specialist, tailored support. The examples of effective cross-community CoSeC support are pervasive throughout the report. Changes to the way CoSeC resource is allocated could be considered to reduce any structural barrier to harnessing synergies for cross-community activity and information sharing within CoSeC and among the communities it supports. **We would like the committee to advise on how the CoSeC resource allocation model could evolve to facilitate the management of CoSeC as pools of expertise. The current EPSRC High End Computing Consortia call provides a specific example to discuss**.

Long term funding of the programme remains an issue. The budget shortfall seen in financial year 2020-21 has continued into 2021-22 with cuts to the programme required to ensure CoSeC can operate within the allocated budget. A flat cash funding allocation has again been indicated for 2022-23 resulting in a shortfall that will be addressed by using a small underspend from 2021-22.

Impact activities continue at pace with the redesign of the CoSeC webpages, the third annual completion of the call for the CoSeC Impact Award, and at the forefront, the migration of individual CCP and HEC websites to new platforms. The CoSeC webpages have been expanded by the addition of some new sections to accommodate new CoSeC activities such blog-posts, and material generated from the CoSeC annual conference.

The recent Physical Science Data Infrastructure (PSDI) Pilot project included a project around data provenance for the BioSim community, which has demonstrated the complementarity and synergy between PSDI and CoSeC. Plans to exploit this synergy are being developed as part of the potential opportunity for a further phase of PSDI. The PSDI pilot ended in March 2022, following on from a statement of needs supported by most of the CCPs and HECs in the community. A considerable part of this Pilot consistent of engagement and consultation activities, led by Barbara Montanari. Most communities supported by CoSeC were consulted via focus groups. A presentation on PSDI took place at the CCP Steering Panel meeting (November 2021) and an update was presented at the recent HEC Chair consortia meeting (April 2022). The long-term aim of the PSDI is to be a tailorable integrated environment, aggregating and automating the processing of data, and combining experimental and simulation data with machine learning methods, to drive integrated, multi-scale physical science to new levels. More generally, as a cross-research-council, cross-disciplinary research-enabling activity, CoSeC is in a very strong position to contribute significantly to a number of the 5 themes of UK Digital Research Infrastructure. Software for research communities and the skills agenda are obvious areas. **We would like to discuss with the committee how CoSeC should evolve to support in the best possible way the aims of EPSRC as well as those of the UKRI DRI in the changed funding landscape.**

A particular success this year is the new resource calculator for applicants to HPC developed by CoSeC staff via HECBioSim. The calculator consists of a containerised backend that will run on the HECBioSim kubernetes infrastructure deployed in the cloud which hosts the data model that is used to forecast HPC time requirements based on parameters known by the scientists, such as system size (atoms), how long they want their simulation (ms), and which code and on which machine. The calculator will then return information on how much system resources are required to run this, thus allowing them to easily calculate compute requirements for RAPs or for other grants. The tool is now available on the HECBioSim website. This is only one example of how a DRI investment could serve to extend the work done for one community so that it could benefit all relevant communities.

The first CoSeC Annual Conference was held in December 2021 as part of the larger Computing Insight UK (CIUK) Conference at Manchester Central Convention Complex. The conference allowed us to showcase some of the work completed within CoSeC and planning is now underway for this year's conference that will again be held in Manchester in conjunction with CIUK. The long-term aim is for the CoSeC Conference to become a stand-alone event in its own right.

A point brought to us by the CoSeC Steering Committee Chair in his role as CCP SyneRBI Chair is around formal agreements around CoSeC work. Until a couple of years ago, a formal Service Level Agreement (SLA) existed between EPSRC and STFC which spelled out the terms by which STFC would provide the CoSeC service in exchange for the EPSRC funding. The merging of Research Councils into UKRI as a single legal entity made the SLA formally void. No other agreement has been drawn up since. CCP SyneRBI have approached us about a formal agreement with them. A better approach may be to re-instate some type of agreement between EPSRC and STFC. **We would welcome some discussion around this point at the upcoming Steering Committee meeting.**

In summary, the specific points where we would welcome advice from the Steering Committee are around:

- **CoSeC's evolution in the changed funding landscape**
- **Allocation model for CoSeC resource**
- **Re-instating a formal service agreement**

Introduction

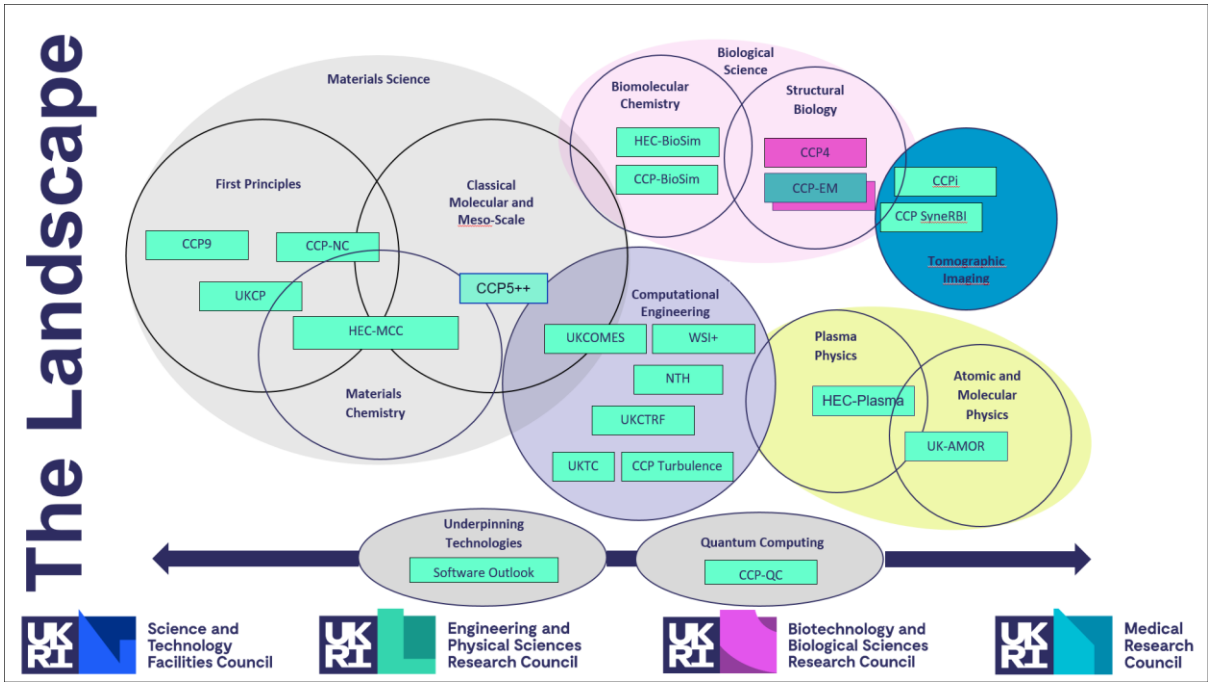
This annual report into CoSeC activities will continue the new reporting procedure agreed at the CoSeC Steering Committee meeting, June 2021, and introduced in the interim report published in November 2021. The aim of this new style report is to present the work of CoSeC over this reporting period – 1 April 2021 to 31 March 2022 – in a more easily digestible format, making it easier to read and understand, whilst maintaining the relevant information.

The report will be divided into the following sections:

- Summary reports divided by scientific area
- Items of significant impact divided by scientific area
- Outline plans for the following year reported by individual CCP/HEC
- An update on resource planning and yearly costing
- Metrics for the reporting period
- Example news items and case studies

The report will also include an appendix for those seeking further information or more detail containing the full individual CCP and HEC reports, as well as updates to the individual CCP and HEC work plans from 2021-22, the individual CCP and HEC work plans for 2022-23, details of code development activity and a summary of training and outreach activities.

The different sections of the report will be grouped together based on the scientific areas identified in the CoSeC landscape diagram below:



Summary Reports

This section of the report will provide summary reports for the 2021-22 year grouped according to the scientific areas identified in the CoSeC landscape diagram. Full reports for each individual CCP and HEC can be found in the appendices to this report.

Project Office

The CoSeC project office continues to operate efficiently and in accordance with the four work packages developed over the last year:

WP1 – Strategy / People / Relations (WP lead Barbara Montanari)
This work package addresses the wider ranging aspect of CoSeC activities including its leadership, interaction with CoSeC communities and funding agencies, and CoSeC's relationship with other national and international computing initiatives for research. The work package will also manage staff development, performance and recruitments.

During this reporting period, the CoSeC Director continued to work as part of the lead team of the **Physical Sciences Data Infrastructure (PSDI, see https://www.psdi.ac.uk). A** Pilot Phase was granted and carried out at short notice between November 2021 and March 2022. This followed on from the Statement of Need, supported by most of the CCPs and HECs communities in addition to a number of other stakeholders, and submitted in February 2021 to the EPSRC call for Large Infrastructure. The long-term aim of the PSDI is to be a tailorable integrated environment, aggregating and automating the processing of data, and combining experimental and simulation data with machine learning methods, to drive integrated, multi-scale physical science to new levels. To this aims, the PSDI will: support multiscale modelling and multimodal research; leverage simulation data to drive experimental science and vice versa; surface data from many sources; provide reference-quality data; standardise, normalise and aggregate data and metadata; enable data to be exploited by AI methods; support workflows that automate data processing; provide a common platform to run models and codes from different sources; seamlessly access performance compute for scaling up; enable software curation and publication; be a place for curation of legacy beyond individual projects. The PSDI Pilot phase achieved the following objectives:

- To engage with the potential PSDI stakeholder community and build the case for its creation
- To undertake some case studies to demonstrate the potential scientific benefits (see details on the PSDI website)
- To trial some relevant technologies and investigate their interoperability
- To gather requirements arising from the case studies and trials and wider consultation
- To analyse these requirements, elucidate the necessary functionality, and propose a technology architecture for PSDI
- To produce a detailed plan for future phases of PSDI
- To create a governance structure for future activities

Extensive consultation was carried out with new and existing communities, including relevant CCPs and HECs. Information on PSDI was presented at the CCP Steering Panel Meeting and the HEC Chairs meeting. The output of the consultation was used to develop an outline plan for the next phase of PSDI, which has now been submitted.

Barbara Montanari continued to serve as member of: DiRAC oversight committee; ExCALIBUR Steering Committee; ExCALIBUR hardware and enabling software working group; CECAM Council; Ada Lovelace Centre Working Group. She also served on number of EPSRC review panels.

She represented CoSeC and the wider Computational Science and Engineering Division she leads at: US-UK AI for science scoping workshop; CECAM meeting on exascale; data-enabled atomistic modelling workshop; CIUK Conference including the CoSeC Conference; Indian DAE-STFC bilateral workshop; Royce data management workshop; MCC community meeting; UK Catalysis Hub meeting. Extensive engagement with the National Centre for Quantum Computing took place.

Barbara was appointed EDI Champion for the Scientific Computing Department, and EDI representative for the National Labs at STFC-wide level. A number of activities are happening, including issuing EDI guidelines for holding events.

CCP Steering Panel and CoSeC Steering Committee meetings were held, and meetings with EPSRC took place to discuss the ongoing financial issues.

Several internal Divisional meetings were held to discuss a number of topics including ML and Accuracy of Potential Energy Surfaces and a meeting to summarise the work completed during the year as well allowing new starters to introduce themselves.

A number of CoSeC staff members were successfully supported through the promotion process.

During the reporting period we have welcomed new staff into the CoSeC programme:

- Kane Shenton joined CCPNC
- Charles Moulinec joined CCPBioSim
- Omar Mahfoze joined CCP-WSI+
- Sai Maganti joined CCP-WSI+
- Donald Chung joined CCPBioSim
- Vendel Szeremi completed some work for Software Outlook
- Alex Skillen completed some work for UKTC

We also saw the departure of Simone Sturniolo, the project lead for CCPNC, with Kane Shenton taking on the role.

A number of staff were coached and supported through the STFC review promotion.

WP2 – Technical (WP lead Stephen Longshaw)
The goal of this work package is to better understand the technical and scientific landscape of CoSeC and create a framework to support its development in a way that is able to evolve. This knowledge will be used to identify overlap between projects, or research. The aim is to facilitate and foster cross-project collaboration and to allow CoSeC to form a leading role in computational science in the UKRI landscape.

To date, this work package has overseen the growth of a number of thematic working groups internally to CoSeC staff around topics like web technologies and scientific code coupling. The former has seen a full technical testbed for alternatives to the current outgoing Drupal 7 platform most CoSeC supported websites rely on and the latter has seen a number of internal technical discussions and led to two publicly available seminars from CoSeC staff members. These are both recorded and available to view online. During this reporting period, this work package has also, in conjunction with WP3, proposed and started the concept of a CoSeC staff blog. This is intended to provide a steady stream of high-level content showing the spectrum of work that CoSeC is involved in, both technical and community-driven.

A steer for CoSeC has that it should look to continue to enhance its leading role in computational science within the UK, offering not just support for its communities but expert guidance on how the

future landscape may look and how to prepare for it. This work package has worked towards creating a new annual CoSeC conference-like event that not only showcases the work of CoSeC staff but also the wider communities that it supports. An initial event was successfully held as part of the in-person conference event "Computing Insight UK" in Manchester in December 2021. The talks were all recorded and are available on the CoSeC website. The event was well received, and work has therefore continued during this reporting period to make it annual. As part of this a new committee has been identified involving both internal CoSeC staff and external community members. An initial meeting of this committee is expected during the next reporting period and will focus on creating an event that stands alone to showcase the cross-cutting topics across the CoSeC landscape.

Alongside the CoSeC conference, the intention is that this work package is also exploring other ways of disseminating the technical work done by CoSeC staff. Within WP3, work to create impact case studies has been ongoing and will continue into the foreseeable future. Within this work package, it will therefore be a priority to help identify key outputs from across the reports CoSeC already generates and help curate a steady stream (aim 6-10) within each reporting period. The hope is that these can then be combined into the form of an annual CoSeC report and published through the STFC library service. This will be explored as an option during the next reporting period.

WP3 – Impact (WP lead Dawn Geatches)

The aim of this work package is to build awareness of CoSeC's valuable role in the scientific landscape of computational research in the UK, increasing its visibility as the hub of a community network for current and future members and funders.

Between April 1st, 2021 and March 31st, 2022 we have published thirteen news articles highlighting the work and achievements of a range of CCPs and HECs, including articles about: the winner and 3 runners-up of the CoSeC Impact Award 2021 (CIA21); the launch of CIA 2022; several collective CCP/HEC news round-ups; the participation of STFC-CoSeC staff in conferences and workshops; and the inaugural CoSeC conference. CoSeC's twitter following has slowed in growth compared to previous years and we now have 244 followers, although there has been a noticeable (but unquantified) increase in the number of 'likes' and re-tweets. With the help of departmental impact sandwich students we held a twitter campaign to advertise the CIA 2022, which also acted as training (for me) in how to construct appealing tweets and target them at relevant audiences. Working with the CIA 2021 winner and runners-up we have published four CIA case studies, and began working on a UKCOMES case study based on its HEC- ARCHER summary report.

Work on the CoSeC webpages continued to the point of publication and since then has been revised based on feedback from the CoSeC Steering Committee and members of CoSeC. We now have an enlarged media section including a blog post (initiated by Stephen Longshaw) and a collection of CoSeC Conference 2021 recordings of talks, and on the CoSeC landing page a direct link to 'Important Information' such as a description of CoSeC's core support (e.g. of relevance to the current HEC call).

The project involving the migration of the CCP/HEC websites from Drupal 7 to a new platform continues with the help of a SCD Computing Apprentice who is funded through Barbara's divisional budget, and supervised by a non-CoSeC-funded SCD staff member. Thanks to the financial contribution of CCPi, we were able to outsource the building of a Wordpress template that we have since copied and are using as the template to customize most of the CCP and HEC legacy-Drupal sites. Some communities have opted to pay the external company to customise and populate the template, while others have opted for the help of the computing apprentice. In the near future there will be the option of central, UKRI web-hosting and maintenance of Wordpress websites, and we are in a good position to take advantage of this when it comes on-line.

WP4 – Project Management (WP lead Damian Jones)

The aim of this work package is to provide coordination through the CCP Steering Panel and programme oversight through periodic reports, and input to reviews, to EPSRC and the SLA Steering Committee, support for the organisation of networking and training events, and manage the progress of the programme staff, L&D and liaise with the communities supported, in particular to help increase the impact of the programme.

During this reporting period the work package has overseen a shift away from the traditional reporting structure based on individual CCPs and HECs towards the new structure seen in this report based on scientific areas as identified in the CoSeC landscape document. This work has included a change to the quarterly project meetings that are now also arranged by scientific field, allowing sharing of information and discussion about potential cross-community activity. These changes are intended to be the pre-cursor to a possible move away from the "OTL silos" that we currently see within CoSeC where people book effort to individual CCPs and HECs and towards the creation of pools of effort within each scientific area.

The costing for financial year 2022-23 (1 April 2022 – 31 March 2023) was calculated, submitted and agreed with EPSRC. Full details of the costing can be found in the "Resource Planning" section of this report.

Materials Science

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

Phase 1 (restructuring of argument list), phase 2 (introduction of types) and phase 3 (error handling) are done. This has resulted in a substantially modernized version of the code having improved workflow, readability, and functionality, and this major milestone has been committed to the public repository. The final phase (phase 4) of the "librification" is currently in progress, 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.

For CCP-NC the main target achieved was hiring a new person to provide support full-time. Kane Shenton took up his role part-time from July 2021, and switched to full-time in October. In addition, work has started on the development of MagresView 2.0, with an initial framework established for a first, basic demo. A beta version, which implements much of the core functionality, is currently being evaluated by users. Work has also gone into developing the theory of dipolar second moments, which has resulted in a script and a paper draft.

In April the annual CASTEP core developers coding workshop (a.k.a. "Codefest") was organised by UKCP and held virtually. 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. An in-person Codefest has been arranged for April 2022.

The release of academic CASTEP 20.1.1 in March 2021 directed users to the new STFC-run licensing and digital distribution service at https://licenses.stfc.ac.uk. During the reporting period 569 research group licences were issued world-wide. CASTEP licensing for academics has been a successful pilot on the platform, which is available for CoSeC-supported projects upon request. CASTEP 21.1.1 for academics was released in December 2021 alongside a revised licence application workflow coordinated with Cambridge Enterprise, who own the IP for CASTEP.

MCC participation in the EPSRC ExCALIBUR programme continued with Ian Bush, Alin Elena and Tom Keal included on the steering group of the Materials and Molecular Modelling Exascale Design and Development Working Group (MMM DDWG). The first phase of the project concluded at the end of July 2021, and as co-Is they have since helped to shape the £2.9m "PAX-HPC" proposal for the next phase. This was successful and is taking forward developments to address the three exascale challenges identified in phase 1 (large scale calculations, complex workflows and I/O), with an emphasis on heterogeneous architectures. They also took leading roles in the community effort to shape the MMM application case studies that are informing these developments, and were co-authors of an article accepted in a special issue of Computers in Science and Engineering detailing these. They organised and participated in meetings with the Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics DDWG which resulted in the two DDWGs identifying commonalities that formed the basis of the combined bid into the next phase, which began in December. A recruitment exercise is now underway for Accelerator Development and Multiscale Workflows PDRA positions funded by the PAX-HPC grant. A PAX-HPC project kick-off meeting was held at Daresbury in March. Ian and Barry have also provided CRYSTAL benchmark cases to the ExCALIBUR exascale challenge problem set.

Benchmarking exercise within MCC focussed on classical Molecular Dynamics, in particular comparing DL_POLY and LAMMPS. An initial set of test cases have been developed, strongly based upon earlier work by Alin Elena, which examine distinct parts of the forcefield, and again with Alin's help appropriate inputs for the two codes have been written. So far work has focused on a simple Sodium Chloride test case, and it has been shown that the two codes can generate the same scientific results over extended runs. As for benchmarking the situation is complex; using runs that generate the same statistical results LAMMPS evaluates the short-range terms and neighbour list more quickly than DL_POLY, while at least when high accuracy is required DL_POLY has an appreciably faster Ewald sum. The net result is that at high accuracy DL_POLY is somewhat faster, while when lower accuracy is allowable the situation is less clear, LAMMPS seems to be faster but this is still being evaluated.

Support of ChemShell development has focussed on enabling use of the Py-ChemShell package on a wider range of HPC platforms, particularly ARCHER2, where efforts to port the code using GNU compilers have now been successful after overcoming a number of issues with the programming environment. An interface to Molpro has been added to enable future excited state and wavefunction-in-DFT developments. Support for the open source version of DL_POLY (DL_POLY 5) as an MM driver has been added, and several interfaces have been updated including LSDalton and NWChem. The 21.0 release was made in December with significantly enhanced functionality and performance.

The software development on DL_FIELD continued to focus on workflows and improving ease of use. This included reprogramming PDB file interpretation within DL_FIELD to achieve a closer integration with ChemShell for setting up QM/MM models for protein systems. On setting up complex multiple potential systems such as organic-inorganic systems, the auto mixing of van der Waals parameters by using Slater-Kirkwood formalism has been implemented. This would allow users to use atomic information such as atomic polarisabilities to derive the Lennard Jones parameters. Version 4.8 was released in September 2021 and included the features mentioned above. After moving the DL_POLY

package to an open source licencing model, the code has been examined for inconsistencies and ported to ARCHER2. MCC have assisted with explaining functionality and looking at side effects in applying radiation damage events.

Biological Science

The Enlighten/ChemShell short project has finished. This adds QM/MM functionality to Enlighten (a plugin to the PyMol visualisation software) which is aimed at making simulations accessible to users who are not experienced computational chemists. The new functionality was demonstrated by Sarah Fegan as part of the Enlighten and ChemShell workshops in the CCPBioSim training week.

The TRex short project began in June. A development server has been provisioned within the STFC cloud and the original Rex server deployed. A code review has been completed and tasks assigned to further develop the platform. The first example software programs have been installed.

The short project "Poseidon" to make the code for calculating entropy through the multiscale cell correlation method available to the wider community has started in September. We have reviewed the existing codes from Richard Henchman's research group and are developing some tests prior to merging the two codes (one designed for proteins and one for solvents). The input parsing functions will need to be rewritten to work with trajectories from recent versions of the MD codes.

The CCPBioSim training week was held online again this year. Participants were able to book sessions individually to suit their interests and schedules. There were an average of 25 people in each session (6 workshops and 2 research seminars). We would like to thank Martyn Winn and Andrea Thorn (CCP4/CCP-EM) for providing the workshop on Validation of Structures from the PDB. Pietro Faccioli (Universita' degli Studi di Trento) and Denise Okafor (Penn State University) gave very interesting research seminars.

In this reporting period a large portion of HECBioSim time has been focused on supporting the community with uptake and access to the national HPC pilot machine ARCHER2 and UK Tier2 JADE2 (Oxford) and Bede (Durham). There has been a large volume of requests across three new machines for support from groups and users when accessing the machines for the first time to achieve performance in production in line with HECBioSim benchmark guidelines. This is mainly due to users being unfamiliar with the new hardware architectures and the benchmark suite tuned to extract even higher performance than previous in a push to raise the bar. These users were all helped to achieve the required performance that they were expecting. To assist with this going forward, more example submit scripts have been included in examples on the website.

A new resource calculator for applicants to HPC via HECBioSim has been developed. This is based on data from real benchmarking data for AMBER, GROMACS, LAMMPS and NAMD on ARCHER2, JADE2 and Bede. The calculator consists of a containerised backend that will run on our kubernetes infrastructure deployed in the cloud which hosts the data model that is used to forecast HPC time requirements based on parameters known by the scientists, such as system size (atoms), how long they want their simulation (ms), and which code and on which machine. The calculator will then return information on how much system resources are required to run this, thus allowing them to easily calculate compute requirements for RAPs or for other grants. This calculator enables beginner PIs and users or non-traditional consumers of HPC, such as experimentalists, to be able to make these estimates and to begin acquiring access. The calculator will also show the energy consumption estimates for the given simulations and rationalise it against things that users can relate to their life (eg number of hours the average family home could be powered). The tool is now available on the HECBioSim website.

Work on Longbow2.0 has started. Longbow2.0 will modernise against the latest standards and trends within the Python ecosystem and introduce functionality in line with recent trends in hardware features available. The original Longbow was written many years ago before these ways of working and technologies emerged. Work so far has been focused on restructuring the original functionality into a more modular library format for better use in other projects. Functionality to support ARCHER2 and better support for machines with GPUs has already been added in. Support for passwords and SSH keys with encryption at rest has also been added, meaning that users of Longbow2.0 will be able to use ARCHER2 (or other very secure machines) without having to enter their password repeatedly. Work on Longbow2.0 has also begun to introduce a lightweight GUI and also shift from defaulting to "persistent monitoring" to "fire and forget" mode.

Computational Engineering

The next planned release of DL_MESO (version 2.8) is currently being prepared by UK-COMES (for Q2 2022) after completion of the full implementation of fluid-filled vesicles (e.g. red blood cells) as a major new feature for the LBE code and addition of new interaction types to the DPD code. Improvements have been made to DL_MESO's documentation with a revamped user manual, a technical manual for user-developers wishing to add their own features to the codes and tutorials with practical guides for new and existing users on carrying out mesoscale (DPD and LBE) simulations with DL_MESO. A newly designed graphical user interface (GUI) based on Qt and Python is being written to replace the existing GUI written in Java and make it easier for users to setup and analyse their DL_MESO calculations.

CCP-WSI+'s parMupSiF partitioned FSI framework has been permanently renamed to ParaSiF. Efforts to develop this framework exist within the CoSeC support for CCP-WSI+ and through other funding initiatives such as the ARCHER2 eCSE programme and the EU H2020 project SLOWD. The goals of the different projects are similar in that they have components of wave structure interaction in their remit, so this represents a good use of resource given the publicly available nature of the framework. Future development of this framework for CCP-WSI+ will revolve around integrating capabilities from the communities existing OpenFOAM based solvers into the interFSIFoam solver. Initially this will focus on the waveFoam solver which is a development of the basic interFoam solver to include enhanced wave generation techniques. In the future this may also include the other major solver related to CCP-WSI+, qaleFoam, which is also interFoam based. However, this is predicated on work being currently performed by STFC CSE staff under an existing ARCHER2 eCSE grant to explore enhancing the overset mesh based coupling approach within OpenFOAM to allow it to be used as part of a partitioned framework based on a code coupling library.

The Multiscale Universal Interface code coupling library is now a core approach within the CCP-WSI+ community (and is the basis for the ParaSiF framework). Significant developments have been made to the library over the reporting period and released to GitHub. The C/Fortran/Python wrappers have all been completely redesigned and are complete and a new top-level CMake build system created for the whole library. As part of a related ExCALIBUR project around code coupling, the parallel performance of the library has been significantly improved, with near-perfect scalability demonstrated on ARCHER2 up to around 1000 nodes.

In order to improve the parallel performance of the CCP-WSI+ OpenFOAM based solvers, a stand-alone decomposePar tool has been created using ParMETIS. This is generally applicable to a number of codes but specifically implemented in a codebase within the CCP-WSI+ code repository. Within the ESI OpenFOAM variant in the CCP-WSI+ code repository, a new capability for dynamic load balancing through mesh refinement has been added. This is under development but represents the foundations

of upcoming improvements to the dynamic load-balancing capability of key solvers within the community.

Development of the CCP-NTH community code, CHAPSim, to increase its numerical accuracy up to 6th order accuracy and to increase its parallel capacity has taken precedence in this reporting period. High order accuracy for spatial discretisation enables CHAPSim the capability to capture subtle characteristics from turbulence and heat transfer with limited numerical dissipation. The multi-dimensional parallelisation makes CHAPSim use the latest advanced HPC systems (i.e. ARCHER2).

During the reporting period, the 'compact scheme' with an up to 6th order numerical discretisation for spatial interpolation, the first and second derivatives has been implemented into CHAPSim. The compact scheme implemented in CHAPSim2 considered both collocated and staggered grid arrangement at various boundaries conditions. The applied compact scheme has been tested in both serial and parallel mode in Archer2. Test cases of solving first derivative and second derivative of given sinusoidal and polynomial functions validated the applied 2nd, 4th and 6th order of the numerical accuracy in both boundaries and the bulk area of the computational domain. All these developed schemes were well integrated with user-friendly application to solve governing equation.

During this reporting period, in addition to the code development, CCP-NTH research study of heat transfer of liquid metal has also been carried out by numerical simulations of flow of liquid sodium in a Y-junction. Three important thermal hydraulic parameters, i.e. the fluid momentum ratio, the temperature differences of two branches and the inlet Reynolds number, were investigated to study their influence on flow development and the mixing characteristics of the flow in the main tube. It is observed that the momentum ratio plays a key role in the mixing flow development and temperature distribution, while the inlet temperature difference has very limited influence on both flow pattern and wall temperature distribution. The inlet Reynolds number has little influence on flow pattern but it dramatically changes the wall temperature distribution. This study of thermal mixing of liquid metal in one of the most widely used pipe junctions reveals different thermal-mixing patterns and thermal stress development under different thermal hydraulic conditions which would benefit the design of robust pipe junctions and valves, and overall safer piping systems.

SENGA+ is one of the key DNS codes in the UKCTRF for studying fundamental flows with simplified chemistry. Time has been spent studying the code to understand its structure by verifying each term in the Navier-Stokes equations and their implementation. Attention has been particularly paid to the implementation of boundary conditions. The objective of the numerical boundary condition is to specify the desired physical boundary condition while suppressing spurious acoustic wave reflections at the open boundaries.

CCP Turbulence oversaw the developments of the STFC-branch of Xcompact3 that has now been merged into the Master branch. A few scalability tests are still necessary to assess that the scalability of the code on ARCHER2. This includes a new installation and testing based on CMake/CTest, a reorganisation of some core subroutines of the code (i.e. the Poisson solver, matrix refinements for stretching in the wall normal direction, adding of new turbulent initialization) and a consistent approach to floating point precision.

The second part of the year was dedicated to porting the code to hybrid architectures with a particular focus on multi GPU(s) porting. This work had been carried out on a mini-app called X3div, which has all the main features of Xcompact3d (high order finite difference compact schemes, FFT solver for the Poisson equation, pressure correction). A first full implementation with multi-GPU offloading is now available which is based on: managed memory management, automatic optimisation of parallel loop

using Fortran parallel paradigms, CUDA aware MPI or Nvidia Collective Communication Library (NCCL) and CUDA FFT for the Poisson solver. A second implementation, exclusively based on openACC, is also available for fine tuning of the optimisation parameters. This version will be mainly useful for cases with large memory requirements.

Tomographic Imaging

In the reporting period CCPi have published two articles on the Core Imaging Library (CIL) documenting the capability of the software and providing use cases. The team has contributed to the submission and review of two other articles using CIL, one published in Journal of Physics D: Applied Physics and one in Nature Scientific Reports. There have also been three releases of the CIL software published in this period adding functionality and addressing issues on the code, versions 21.1.0 and 21.2.0., 21.3.1.

The first prize in the CoSeC Impact Award 2021 was awarded to Ryan Warr from University of Manchester, for his work supported by CCPi: SCD Winners of the 2021 CoSeC Impact Award (stfc.ac.uk).

On 20 May 2021 CCPSyneRBI released SIRF 3.0, on 24 June 2021 SIRF 3.1 and on 6 July 2021 SIRF 3.1.1. In these versions of SIRF, they updated versions of software packages on which SIRF depends and incorporated new functionality, with highlights preliminary support for the PET data of the GE Signa PET/MR scanner and additional GPU projectors for PET. These releases also contain contributions from the community (merged with assistance from CoSeC) and in particular the support for our first non-Cartesian MR sequence.

The 8th CCPSyneRBI – CCPi joint Hackathon took place on 23 to 26 November 2021, with face-to-face sessions in Cosener's House, Abingdon on 23 and 24 November followed by online sessions on 25 and 26 November. The goal of this hackathon was to establish a benchmark between the numerous iterative algorithms for CT and PET reconstructions that have been proposed in the recent years, with a focus on randomized algorithms. Such algorithms would be developed within CIL and make use of SIRF for PET data. There also was a group working on subset data structures in STIR to enable efficient computation on subsets of PET scanner data. A second part of the hackathon was planned for early April 2022.

A consistent effort is made in outreach and several training sessions have taken place for both CIL and SIRF, utilising the STFC cloud jupyter hub. The largest event was attached to the Fully3D international conference, which saw the participation of 50+ trainees in a remote setting, and took place in 3 weeks from the 28 of June to the 16 of July 2021. The CCPi team has also run two additional training days, one in September at the ToScA (Tomography for Scientific Advancement) and one on the 15 December, with 13 and 26 trainees respectively.

Additionally 3 presentations at CIUK and IBSim-4i conferences and Manchester Ideas forum about CIL have been done by the CoSeC team.

The latest version 3.2.0 of SIRF was released on 22 March 2022. It is the first SIRF version that is capable of handling non-cartesian MR encoding trajectories: 2D radial, golden-angle increment radial and stack-of-stars, and exposes advanced parameters from STIR RayTracingMatrix object to SIRF C++ and Python interfaces.

Atomic and Molecular Physics / Plasma Physics

A main highlight of the year was the (13-15 April 2021) joint UK-AMOR (and CCPQ) – CCP/HEC-PLASMA workshop, 'Atomic and Molecular Data Needs for Plasma Applications', with ~160 registered participants, 23 talks, 3 informal discussion sessions, a demonstration by Quantemol Ltd and a poster

session. The posters and talks are preserved on the CCPQ website and a summary proceedings document is planned to be made available.

Martin Plummer applied and secured STFC Ada Lovelace Centre funding for a 6-month placement for an STFC Graduate Employee to work on the UK-AMOR RmatReact theory (and code), September 2021 to March 2022, in preparation for introducing rearrangement channels (reactions) into the package. Martin has also worked with PI MM Law (Aberdeen) on a proposal to adapt and use RmatReact for low-energy antimatter, specifically anti-H collisions with molecular hydrogen of direct relevance to the CERN ALPHA project (co-I Martin Plummer, project partners J Tennyson and M Charlton (Swansea and ALPHA)). This proposal is now ready to be submitted in June 2022. The Graduate project (supervised by Martin Plummer) has been a great success and informed the proposal, investigating the combination of mixed and single-system Jacobi-like coordinates needed for rearrangement R-matrix collisions: the future application of the work to CERN experiments was the main reason the Graduate project was funded.

Quantum Computing

Alin Elena was part of the organising committee of the Integrating Quantum Computers in Condensed Matter Physics Simulations, National Physical Laboratory, 23-24 September 2021 with invited speakers Professor Viv Kendon (University of Durham), Dr Tom O'Brien (Google), Professor Emanuel Gull (University of Michigan), Dr Panagiotis Barkoutsos (IBM Europe, Zurich), Professor Mónica Benito (University of Augsburg, Germany), Dr Ash Vadgama (National Quantum Computing Centre). The event was hybrid with 120 attendees online and 25 in person in the NPL. A follow up workshop will happen next year in Manchester at the European Physics Society conference. Alin was also invited at the ground breaking ceremony at the National Quantum Computing Centre site at Rutherford Appleton Laboratory.

CCP-QC working group 2 "Crystallography and Quantum Mechanics" was part of the CoSeC Conference held at Computing Insight UK 2021 in Manchester where progress was presented. Working group 3 was established, with Dominik Jochym concentrating on "Quantum Computing and Electronic Structure".

Underpinning Technologies

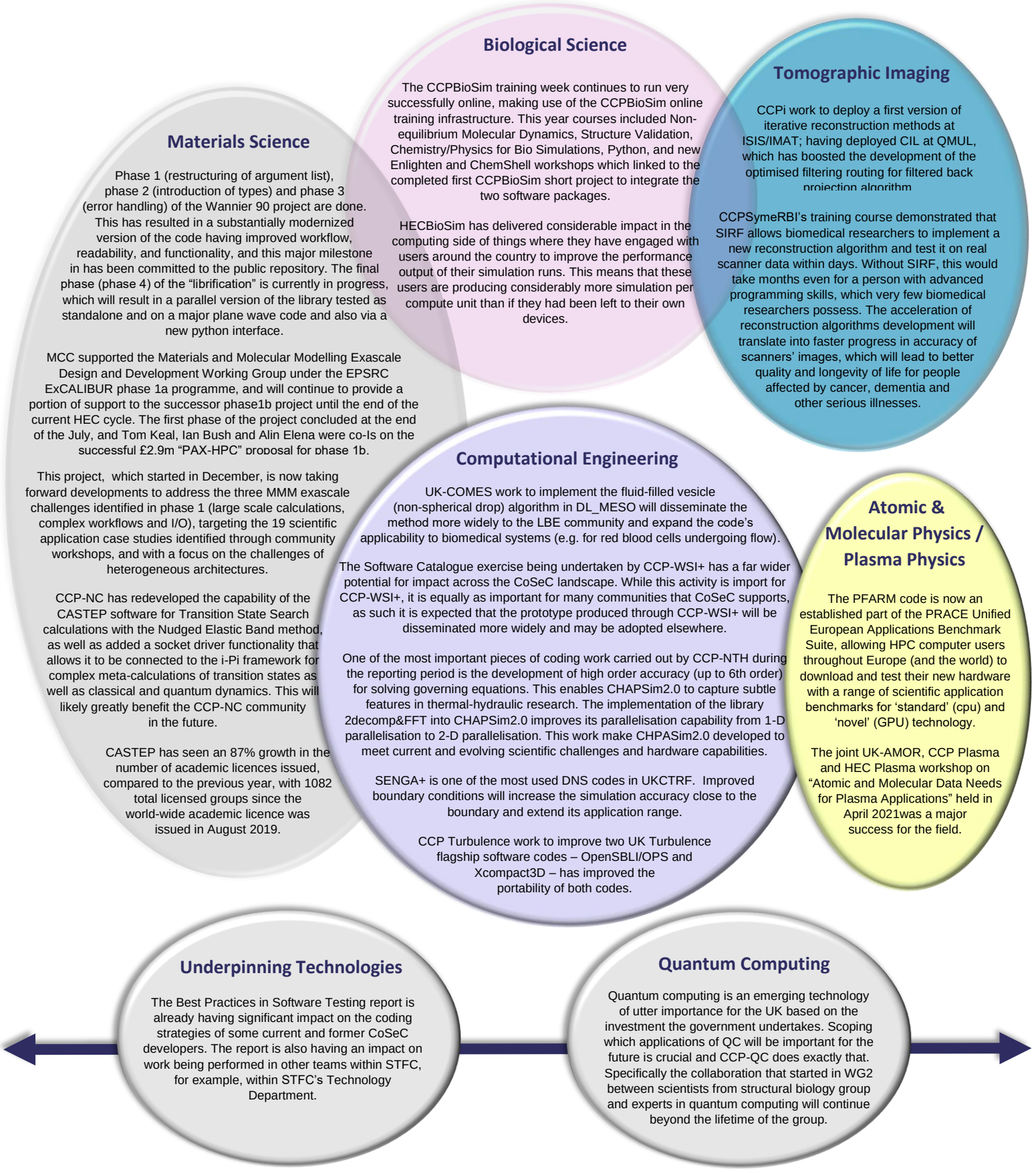
The Software Outlook work plan was reduced significantly during this reporting period to accommodate the FTE deficit within CoSeC. Activities removed included five months planned work on "AI Chips for HPC" with Graphcore and an update to the last software audit.

Software Outlook's latest best practice guidance report has been released, focussing on software testing. This guidance will allow CoSeC Developers to focus their software testing efforts in the manner most suited to their projects and available resourcing: to ensure that the software is reliable and serves its purpose, it is important that a structured testing strategy is used.

As part of the CoSeC Working Group on Code Coupling, Philippa Rubin gave a seminar on the Software Outlook Code Coupling work, which was well received. She has completed the accompanying report, which is also available via Software Outlook's Code Coupling webpage. A technical report was also released summarising the different frameworks available for exploiting hybrid (CPU+GPU) architectures and comparing them.

Impact

In this section of the report we highlight some areas where the work of CoSeC during this reporting period (1 April – 30 September 2021) is having an impact in our communities, across our communities and further into the general public domain.



Outline Plans 2022-23

This section contains the individual outline plans for 2022-23 for the CoSeC supported CCPs and HECs.

Project Office

Funding of the CoSeC programme remains one of the main issues to be addressed by the Project Office over the next few months and continued discussion with EPSRC will help to map out what the funding for future years could look like. The Project Office will continue to explore the change from working in defined CCPs and HECs to working within scientific fields as outlined in this report. The quarterly project meetings will continue to explore the possibility of cross-community work and sharing of expertise and knowledge across the communities.

On the impact side the redevelopment of the CoSeC website is a major task, as is the supervision of the migration of CCP and HEC websites from Drupal 7 to their new platforms. The CoSeC Annual Conference will move into its second year as a stand-alone event and we will explore the possibility of a dedicated journal edition to disseminate the information and material from the conference. We will also look to identify and facilitate the start of new thematic working groups and the continuation of current groups.

Materials Science

CCP9

The Wannier90 programme will be concluded, the BSE-susceptibility study will continue with DMFT, and depending on new hire we will start working on the Casino or ONETEP project. Software engineering will focus on Compton profiles and CRYSTAL parallelization.

CCPNC

While plans for 2022/23 are not finalised (the objectives are set at 6-monthly Steering Group meetings), the proposed work for 2022/23 will be aligned with the work packages of the current funding period for CCP-NC.

- Maintenance and expansion of core tools: publicising of MagresView 2.0 (WP1.1a), developing publications around Magres database (WP1.2), maintenance of Soprano and reimplementation of Magres Python within it.
- Software renewal project: re-implementation of SODORG code, as approved by Steering Group (original WP1.1b & WP1.3a).
- Focus on user engagement, building on strategy developed in Oct 2021–Apr 2022 WP2.1–WP2.3).
- Industrial Engagement PDRA position (WP3) will start in 2022 (funded for 18 months). This is expected to involve placements in three distinct companies.

UKCP

Management and maintenance of the CASTEP code base, continuous integration testing, licensing and distribution to users is the core of CoSeC support for UKCP. Particularly to allow UKCP member groups working on CASTEP to focus on algorithm development and scientific output. A revised CASTEP interface to a popular 3rd-party library of DFT approximations, libXC, has been developed with Durham, Warwick, York and STFC-RAL. We plan to extend existing advanced spectroscopic simulation methods in CASTEP to make use of the library.

MCC

Benchmarking: The benchmarking effort is based upon the principle that code comparisons only make sense if the two or more codes are producing the same scientific results, as only then can researchers

really choose the most efficient application for their work. To this end the work comparing simulations employing only non-bonded interactions in DL_POLY and LAMMPS will be completed, before moving to work on the bonding interactions. Subsequent to that it is proposed that DFT codes are examined, with CRYSTAL and CP2K being possibilities.

CRYSTAL: CRYSTAL22 is currently due to be released Q1 in 2022, and we shall support that effort and make the new release available to MCC users as early as possible. One of the main factors in the performance of CRYSTAL is the distributed matrix diagonaliser. Currently SCALAPCK is employed, but due in part to the various exascale efforts worldwide several alternatives are available. We shall examine their performance in CRYSTAL, initially focusing on ELSI.

ChemShell: ChemShell development will continue to focus on the new Py-ChemShell code. The embedded cluster model for covalent materials will be extended to the hybrid MPI/OpenMP QM code LSDalton, to assess if this offers greater performance on platforms such as ARCHER2. An interface to the MolSSI basis set library will be added to simplify input of basis sets in QM calculations. New DL-FIND algorithms (e.g. GPR) will be integrated into the main release and validated for materials systems. Py-ChemShell will be continued to be maintained on ARCHER2 and Tier 2 systems such as UCL's Young facility, together with the legacy Tcl-ChemShell package. The planned functionality and usability improvements complement proposals submitted to EPSRC for development of predictive methods for hybrid catalysis (with UCL and Bristol), and support for surface science research communities including MCC (with Cardiff and Warwick). The ChemShell effort allocation also covers Tom Keal's work as CoSeC lead for MCC support.

DL_POLY: The package support and development will continue to focus on performance enhancements in collaboration with Ian Bush and special features for ChemShell and radiation damage studies. Enhancements will aim to speed up short-range evaluations and the special feature will be all-all coulombic evaluations and full frozen-frozen interactions evaluations based on systolic loops.

DL_FIELD: The software development will continue to focus on workflow and improve ease of use, especially in setting up complex system models. DL_FIELD capabilities and usages will be significantly broadened to include capability to read third-party force field file formats that can integrate with all other force field schemes already implemented within DL_FIELD. For instance, capability to read CHARMM's rtf files. This extends DL_FIELD capability to access to third party force field webservers such as LigParGen, SwissParam, for novel molecules force field setup..

Biological Science

CCPBioSim

We will continue our short software projects creating or improving software for the biomolecular simulation community. Each project will be focused on making a tool available to the wider community or adding functionality to an existing tool. A call for proposals to the community will go out in the autumn. A prioritisation exercise will be carried out for former flagship projects, legacy software and completed short projects, in order to create a sustainable long-term support plan for them. We will organise training activities including the CCPBioSim Training Week and contributing to the CCP5 Summer School. The Industry Seminar Series is expected to continue. The 5th Manchester Multiscale conference will be organised for spring 2023.

HECBioSim

The 2022/23 year will continue to see large volumes of users with workloads split across a number of different hardware architectures and with this comes a long tail of support. Activities will continue

to focus on supporting consortium members with exploiting HPC at all levels which involves a combination of direct support, training, performance benchmarking documentation. Support will continue for PI's written project proposals and to the HECBioSim RAP panels in the form of technical assessments to optimise resource allocation based on software and hardware suitability matching. There are a number of software development projects that we will engage with and bring under support of the consortium long term. Development of Longbow 2.0 will continue with a release expected around mid-year and this will enable ease of use of HPC in a system agnostic way for consortium members. We will also widen participation in benchmarking amongst the codes we "support" for HPC access and scope development projects in improving access to and performance of AI and large scale ensemble sampling.

Computational Engineering

UK-COMES

The major task for DL_MESO during the upcoming year will be to create a HiLeMMS interface for its LBE code (DL_MESO_LBE). This will enable DL_MESO_LBE to interface with and couple to other solvers, vastly expanding the range of simulations the code will be able to carry out and unifying the user experience with that of MPLB.

Two major tasks are scheduled for the HiLeMMS interface. Exploring the integration of the AMReX code for an adaptive mesh refinement (AMR) capability will greatly enhance the capability of the LBE method to simulate multi-scale real-world flow problems. The C++ template metaprogramming technique will also be explored to enhance automated integration of contributions from research communities for new functionalities, encouraging more contributions from these communities.

CCP-WSI+

The CCP has a goal to produce a general, extensible and accessible coupled framework for all WSI-type problems. This is an ambitious goal but one that is well underway in the initial form of the ParaSiF framework, plans over 2022/2023 build on this general framework to integrate CCP-WSI+ community-specific codes and help the community to deliver this extended framework widely. 2022/23 will also see significant changes to the CCP-WSI web platform, a subtle but important piece of work, this will also tie in to the release of a protoype of a new Software Catalogue. Finally, important performance related topics such as dynamic load balancing will continue to be explored and implemented in appropriate software such as OpenFOAM, this will feed directly back into the overall WSI software framework.

CCP-NTH

The main community building and networking activities included a one-day special topic workshop (quarterly), a one-day cross-CCP workshop and a one-day annual technical meeting. The main training is the annual CHAPSim users' meeting and training courses.

UKCTRF

SENGA 2 is a sister code of SENGA +, which is a dimensional code with detailed chemistry. Implementing the transverse and diffusion terms in the NSCBC boundary condition for SENGA 2 will improve the performance of the code and increase the simulation accuracy close to the boundary. HAMISH is a new generation code in UKCTRF. The performance of the code will be tested in ARCHER2.

UKTC

Funding for UKTC is currently due to end in 09/2022. If funding is available, we will continue to investigate the integration of particle tracking into Xcompact3d, subject to agreement with S Laizet.

CCP Turbulence

The major task for Xcompact3d will be to merge the GPU porting of the mini-app into the main branch of the code to properly take advantage of the code development also in production calculation. The second main task for the code development is to add openMP offloading to both multi-core CPU and GPU to complement the work already done with openACC.

For the OPS code, the major task will be developing the linear algebra solver as well as the OpenSBLI codes for generating the codes for implicit schemes. Together with this major task, we are going to gradually take more responsibility on managing the code development workflow.

Tomographic Imaging

CCPi

In the next year we 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, such as ISIS/IMAT, CLF/EPAC and QMUL, for instance. An important addition to the CIL, i.e. the new filter-back-projection algorithm has been pushed by the interaction with QMUL.

The team is supporting different institutions to embed the required solutions in their workflows. This is achieved by regular meetings with the CoSeC team and the customer.

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. The training on the DVC code is being prepared with the support of Oregon University. A training session on the cross platform build system CMake is run bi-yearly, though a yearly event would be more advisable.

CCPSyneRBI

In 2022/23 we plan to make further additions to SIRF, in particular, handling more MR sequences, PET Time-Of-Flight support and creation of gated sinograms from the listmode data. We will also expose STIR functionality for list mode reconstruction. Finally, we will consider options of computing gradients and values of MR objective functions, PET-MR reconstruction using Python tools/toolboxes and the creation of example interfaces to Machine Learning framework(s), based on initial work at UCL.

We will restart the work on the XNAT database integration, providing sample pipelines for image reconstruction via docker integration between XNAT and SIRF. This work had to be put on hold due to resource reduction, but is now raised in priority by the SyneRBI Steering Panel.

On the general maintenance front, we will complete installation via conda, and continue effort on code optimisation, including use of GPU computing.

Atomic and Molecular Physics / Plasma Physics

HEC Plasma

HEC PLASMA does not currently have active CoSeC support in 2022-2023 due to lack of staff availability (this may change during the year). The consortium may well apply for new support in the Renewal Call. In this case detailed plans for CoSeC support will be made then. In the meantime, UK-AMOR support will look out for further opportunities to follow up the joint meeting on plasma applications of atomic, molecular and optical physics.

UK-AMOR

CoSeC UK-AMOR support is continuing at 0.2FTE through 2022-2023 until the result of the HEC Renewal Call is announced. In Q2 and Q3 of 2022 the main focus for CoSeC UK-AMOR support will be to support the UK-AMOR proposal in the two stages of the application and, in Q2, agree detailed support plans at a higher level of funding. General support will also continue to look for new funding (including support for an ongoing application for studies of antihydrogen molecule collisions led by Aberdeen University) and continue to augment ongoing research funded through other grants and ARCHER2 eCSE projects, as detailed in the milestones. Plans for Q1 2023 and 2023-2024 at the planned higher level of support will be set out in the half-year report (September 2022) following the proposal submission. A full programme of support/collaborative activities will be set out across the range of UK-AMOR codes and activities, to complement ongoing grants and new research proposals by UK-AMOR members.

Quantum Computing

CCP-QC

Plans are to finalise the current working group work around crystallography and kickstart a DFT working group work. We will also liaise with the National Quantum Computing Centre and other CCPs to create a Quantum Computing for Computational Scientists training and informing event in Q1 2023.

Resource Planning

This section of the report outlines the financial details and resource planning for 2021-22 and looks ahead to 2022-23.

Information redacted.

Metrics

This section of the report includes the CoSeC metrics for 2021-22.

The metrics currently used for this programme are defined as:

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

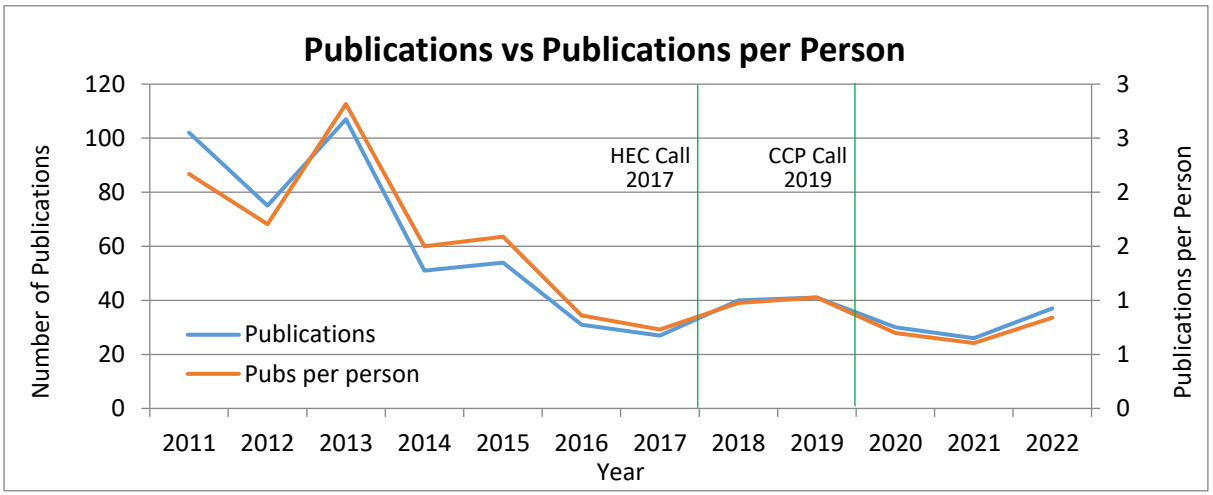
The metrics are per financial year, with the exception of the citations metric, which is for calendar year (for ease of data collection). In the metrics graphs below, the blue line refers to the total number while the orange line refers to the number per scientific/technical staff member. This is useful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

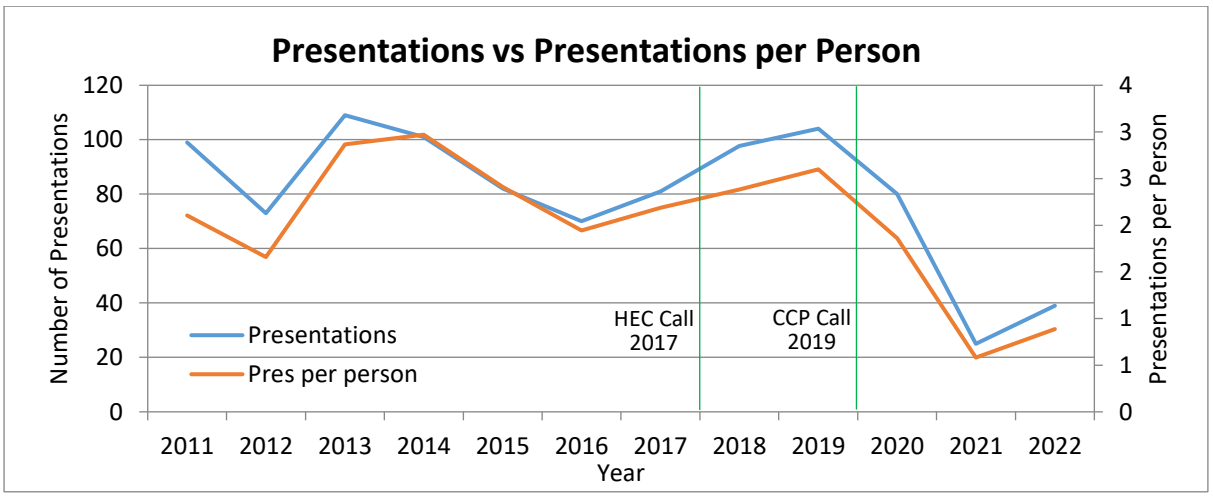
Metrics breakdown by area

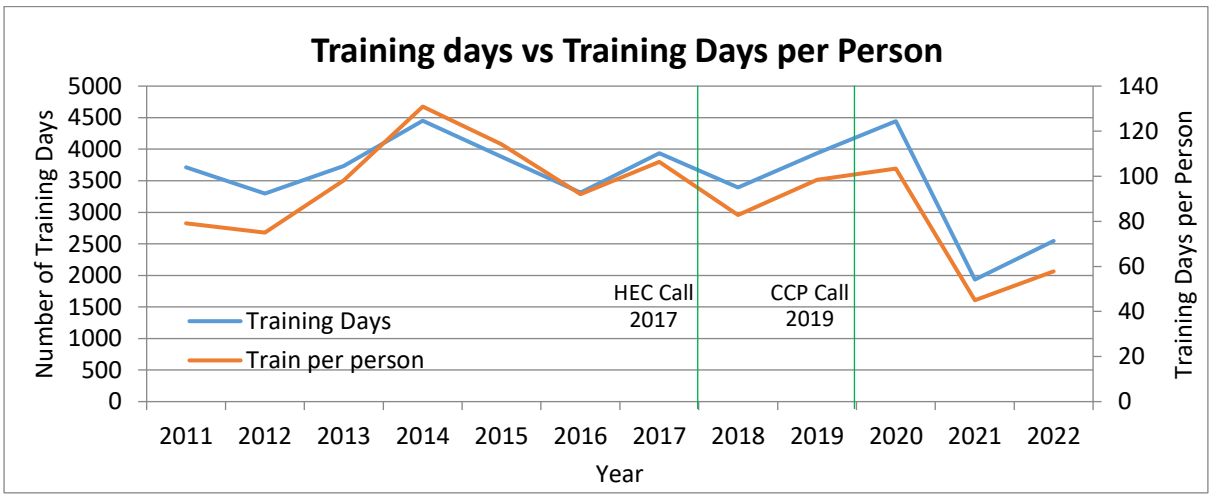
	FTE	Publications	Presentations	Training Days	Citations
Materials Science					
CCP9	3.00	1	4	560	250
CCP-NC	1.40	0	0	0	39
UKCP (including CASTEP)	1.00	1	0	0	1882
MCC (including ChemShell, CRYSTAL)	2.00	6	9	148.5	708
Biological Science					
CCPBioSim	1.95	1	6	331	12
HECBioSim	0.80	1	0	0	0
Computational Engineering					
UKCOMES	0.60	1	2	128.5	25
CCP-WSI+	2.00	6	5	50	90
CCP NTH	1.00	3	1	59	0
UKCTRF	0.50	0	0	0	0
UKTC	0.40	3	3.5	37.5	0
CCP Turbulence	1.75	3	0.5	37.5	0
Tomographic Imaging					
CCPi	1.50	4.5	4	304	0
CCP SyneRBI	1.80	2.5	1	225	14
Atomic and Molecular Physics / Plasma Physics					
HEC Plasma	0.20	1	0.5	240	68
UK-AMOR	0.20	1	1.5	320	102
Quantum Computing					
CCP-QC	0.60	0	0	0	0
Underpinning Technologies					

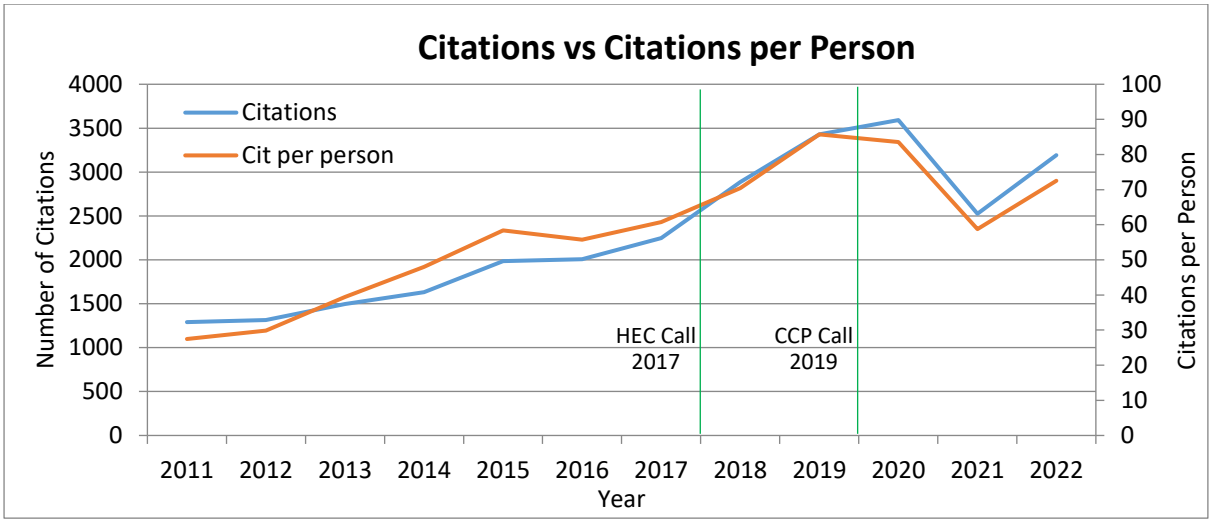
Software Outlook	1.50	3	1	104	1
Totals		**38**	**39**	**2545**	**3191**

NOTE: fractional figures arise due to cross-project activities where the metric is shared between multiple projects.








Citations vs Citations per Person
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CCP Call 2019
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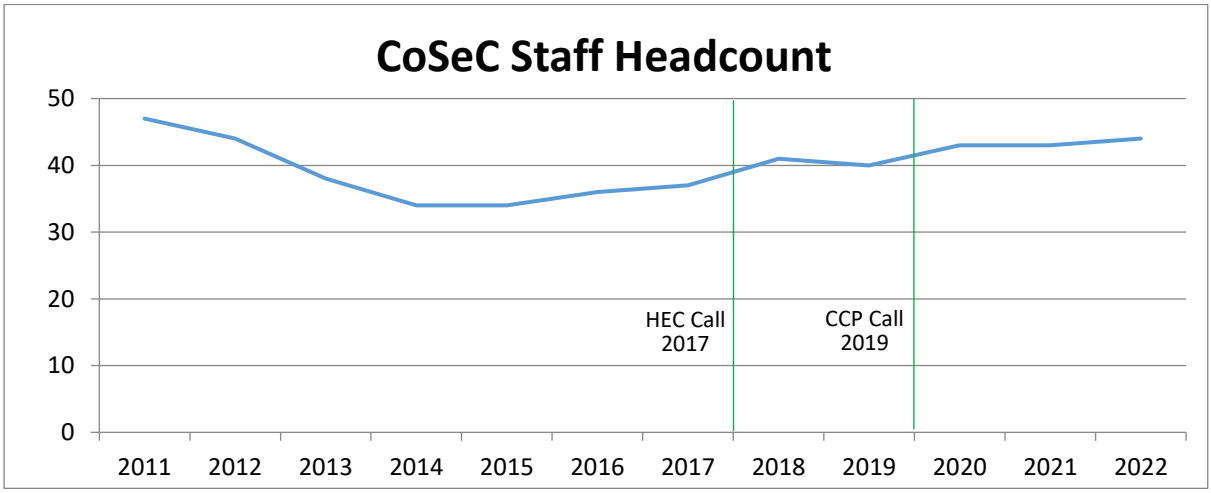
CoSeC Staff Headcount
HEC Call 2017
CCP Call 2019
50
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30
20
10
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2011
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2013
2014
2015
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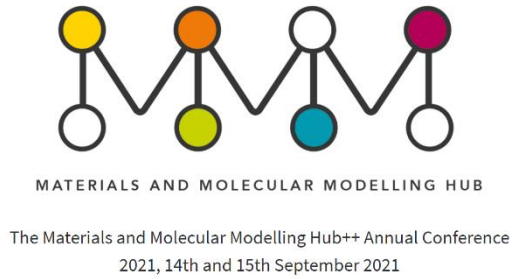
2017
2018
2019
2020
2021
2022

CoSeC News Items and Case Studies

This section of the report includes a small example of news items and case studies from 2021-22.

CoSeC Communities Collectively Collaborate (Published 28 Sep 2021)

CoSeC staff and their communities have been busy supporting conferences and workshops.



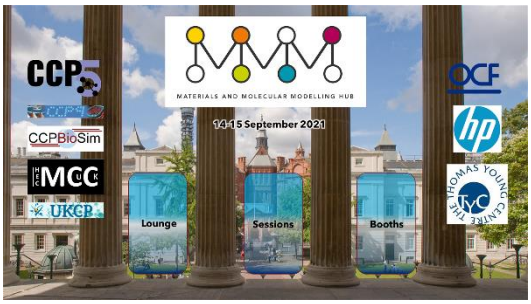
"Possibly the most ambitious conference in materials and molecular modelling ever organised in the UK, at least I can't think of another that comes close in the past 20 years";

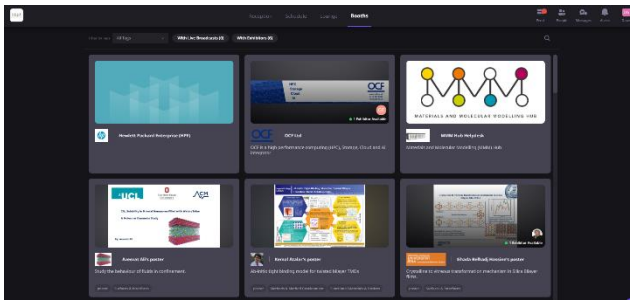
"I think that the distribution of attendees at the parallel sessions reflects the proportion of groups working in the respective areas. It is indeed promising to see so much interest in the new methods and method development! It's a sign of the vitality of the community".

The above comments were made by members of the organising committee of this year's online, 2-day MMM Hub ++ Conference about materials and molecular modelling and high performance computing, and they reflect the conference's success and the strength of the support shown by the community of researchers and developers in this field.

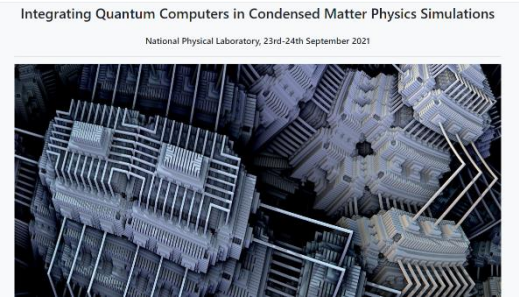
The MMM Hub and Thomas Young Centre, together with the Collaborative Community Projects (CCPs): CCP5, CCP9, MCC, UKCP and CCPBioSim, organised the conference. STFC's Dr. Alin Elena was part of the organising committee and chaired two of the 'Surfaces and Interfaces' parallel sessions, with others led by delegates or chairs of the supporting CCPs.

Dr. Andrey Brukhno (STFC) gave a presentation: "Interscale Simulation: a Novel Combined Methodology to Bridge Between Scales and Methods in the session 'Biomolecules and Biological Soft Matter", which was one of three parallel thematic areas on the first day. The first afternoon was dedicated to providing a platform for Early Career Researchers to present their research.





Overall, the conference attracted more than 250 participants from 17 countries across the world including Mexico, Iraq, Russia and Australia. Above are screenshots of the virtual conference including the entrance portal (left), and the booths for posters and exhibitors (right).



Dr. Elena was also on the organising committee and a session chair of the hybrid online and in-person workshop: 'Integrating Quantum Computers in Condensed Matter Physics Simulations', held over two days at the National Physical Laboratory, London. Supported by CCP5, CCP9, CECAM Daresbury node and NQCC, the aim of the event was to '....bring together experts from the quantum computing community with

experts in condensed matter to give an overview of the field and of current developments, and to generate ideas for further quantum computing applications within condensed matter physics.'

Approximately 120 participants overall (including 25 venue attendees) listened to the talks given by invited speakers including Prof. Viv Kendon (Chair of CCP-QC), Dr. Tom O'Brien (Google), and Dr. Panagiotis Barkoutsos (IBM).

Expanding and extending networks both personal and community based (Published 08 Oct 2021)

Dr. Wei Wang (pictured left) of STFC has been awarded the prestigious status of 'Visiting Scholar' in the Department of Mechanical Engineering at the University of Sheffield, from 13th October 2021 to 31st March 2025. As the secretary of the Collaborative Computational Project in Nuclear and Thermal Hydraulics (CCP-NTH[1]), and the main developer of the CCP-NTH Community code CHAPSim[2], Wei supports a community of researchers and engineers to develop and maintain computational methods and software packages to modernise the nuclear thermal hydraulics tools. These computational methods and software packages are designed to meet the demands imposed through the development of advanced, next-generation nuclear reactor systems that are scheduled for deployment in the coming decades.

In addition to enhancing the work of CCP-NTH, Dr. Wang's appointment builds and strengthens links between STFC's Computational Engineering Group[3] and Prof. He's Group (Dept. of Mechanical Engineering, University of Sheffield).

Official Launch of CCP5++

September 29th saw the official launch of the CCP for Integrating Computer Simulation of Condensed Phases with experiments and data science[4], CCP5++, which builds on the successes of CCP5, the CCP for Computer Simulation of Condensed Phases[5]. The new network grant was launched with an invite-only meeting including participants Prof. Sir Richard Catlow, vice president of the Royal Society and former CCP5 chair, and Prof. Ignacio Pagonabarraga, director of CECAM[5], Prof. Jonathnan Rowe of the Alan Turing Institute, and Prof. Peter Haynes of the Royce Institute and Psi-K president. Prof Paola Carbone of the University of Manchester is the Principal Investigator of the network and Dr. Alin Elena of STFC is the Secretary and Co-Investigator.

1. CCP-NTH aims to develop a strong, collaborative community in nuclear thermal hydraulics
2. CHAPSim is a A **CH**annel **A**nd **P**ipe flow **sim**ulation solver, *CHAPSim*, is an incompressible Direct Numerical Simulation (DNS) code for flow and heat transfer with MPI parallelization
3. Computational Engineering Group combines leading-edge expertise in scientific modelling with the latest high-performance computing to solve complex and leading-edge engineering problems
4. CCP5++
5. CCP5
6. The (CECAM) Centre Européen de Calcul Atomique et Moléculaire node at Daresbury Laboratory is hosted by STFC's Scientific Computing Department (SCD)

CoSeC Impact Award 2021 Winner (Published 8 Oct 2021)

Improved Images emerge from the 4th Dimension

CoSeC
Computational Science Centre for Research Communities

At the time of winning the CoSeC Impact Award (2021) Ryan Warr was a 3rd-year PhD student in the Henry Moseley X-ray Imaging Facility at the University of Manchester, where his research concerns the advancement of Spectral X-ray Computed Tomography imaging techniques. Ryan built on and developed existing imaging software to improve the quality of X-ray images by extracting the maximum amount of relevant information from poor quality images. The research aids the precise identification, visualisation and analysis of materials, enabling advanced imaging across fields including medical imaging, geology and security scanning.

Background

For many years, X-ray computed tomography (CT) has been used to non-destructively obtain insight into materials and objects, collecting sets of 2D images and recombining them to produce a detailed 3D map using a reconstruction algorithm. These techniques have been applied in a wide range of fields, including medical imaging, materials science, industrial testing, etc.

Conventionally, X-ray detectors produce 'black and white' images, where higher density objects (e.g. bone) will appear brighter than surrounding, lower density materials (fat, muscle). Where materials have similar density (e.g. soft tissue), however, the contrast between them, and hence structural detail, is poor. One way to address this is to use hyperspectral detectors.
On interacting with X-ray photons, every chemical element emits a unique, identifying spectral signal corresponding to a specific energy that can be used as an element's 'marker'.

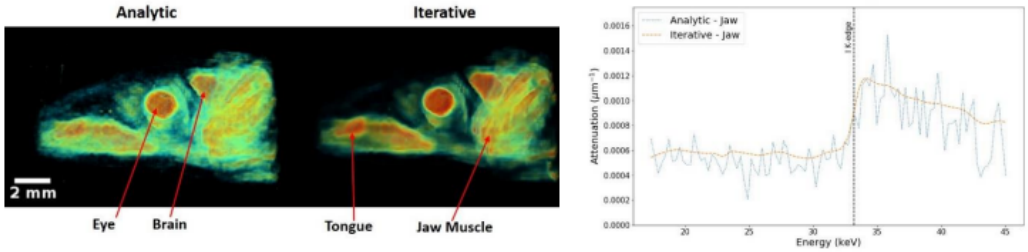
With hyperspectral detectors, the exact energy of any markers can be precisely identified and used as fingerprints, confirming the presence and position of an element within the sample.
Hyperspectral tomography is a relatively new technology, and a number of challenges must still be overcome to optimize the data obtained from the imaging method.

Challenges

Hyperspectral imaging unlocks access to an additional layer of energy-based information, yet current detector technology is still in its early stages. More demanding signal processing limits the amount of data we can collect during imaging. One may compensate for this by imaging for longer, but in some cases time or X-ray dose is restricted. The consequence is each image often suffers from poor signal-to-noise ratio, making structural features harder to distinguish. For spectral images, the unique energy markers may be hidden by noise, limiting the ability to map chemicals by their fingerprints. The correct choice of reconstruction algorithm is therefore crucial to counteract such issues and restore optimum image quality. Standard, analytic reconstruction methods typically fail to suppress high levels of noise. Advanced, iterative algorithms offer a solution but their availability is limited and inconsistent.
Therefore, it is essential to develop novel algorithms for optimum spatial and spectral image quality.

Ryan's role in addressing the challenges

Ryan has used the flexibility of the tomographic imaging open source software: Core Imaging Library (CIL), to create and test a novel, dedicated iterative reconstruction algorithm that can suppress noise and restore feature definition to key structures. With hyperspectral data, there are many similarities observed across the spatial and spectral dimensions. While this information cannot be utilised by analytic routines, an iterative algorithm can exploit such structural correlations to improve reconstruction quality. Ryan's PhD work involved the optimisation and application of the novel algorithm to reconstruct 4D (3D spatial + 1D spectral) datasets of stained biological specimens. The chemical agents used for staining are often low in concentration and inhomogeneously distributed, made worse in the case of noisy data. Novel iterative methods can successfully overcome such issues, enabling excellent characterisation and visualisation of chemically-stained soft tissue regions. The development of such algorithms to aid elemental analysis has the capability to improve the insight and understanding of samples within biology, geology and industrial testing.



Left: Noise reduction and improved chemical mapping of iodine stain in soft tissue using iterative method.
Right: Application of smoothing method to energy profile within jaw of sample, significantly reducing noise.

CoSeC's Impact

"Through CoSeC, my understanding of designing and optimising reconstruction algorithms has grown immensely by working closely with the CCPi. Being able to share and communicate new ideas through 'hackathon' and workshop sessions has vastly improved my theoretical knowledge and coding skills. I hope to continue my research in hyperspectral imaging and help to advance it across a wide range of applications, including geology, bio-imaging and non-destructive testing. As the imaging hardware, and software innovations such as CIL, continue to improve, I can only see hyperspectral imaging becoming more commonplace and I hope to be there when it does!"

Ryan Warr

CoSeC's network of supported communities enables invaluable opportunities to work across the Computational Collaborative Projects (CCPs) including CCPi - for Tomographic Imaging. CCPi aims to provide the UK tomography community with a toolbox of algorithms that increases the quality and level of information that can be extracted by computed tomography.

www.cosec.stfc.ac.uk

@CoSeC_community

Funding: This work has been enabled by the EPSRC grants: EP/M022498/1 and EP/T026677/1. Ryan also acknowledges support from the European Research Council grant No. 695638 CORREL-CT.
Further information: An article was accepted for publication in September 2021, discussing the application of novel iterative algorithms to lab-based hyperspectral X-ray CT datasets.
Further papers describing the background and basic use of the CIL software (see https://www.ccpi.ac.uk/CIL)

UKRI Engineering and Physical Sciences Research Council
UKRI Science and Technology Facilities Council
CCPi Tomographic Imaging
MANCHESTER 1824 The University of Manchester

Financial Year 2021-2022 Annual Report

(*Covering the period 1 April 2021 – 31 March 2022*)

APPENDICES

Appendix - Individual CCP/HEC Reports

This appendix contains the full, individual summary reports for 2021-22 for the CoSeC supported CCPs and HECs.

Materials Science

CCP9

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

Phase 1 (restructuring of argument list), phase 2 (introduction of types) and phase 3 (error handling) are done. This has resulted in a substantially modernized version of the code having improved workflow, readability, and functionality, and this major milestone in has been committed to the public repository. The final phase (phase 4) of the "librification" is currently in progress, 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 CoSeC team has weekly discussion sessions, and progress/future tasks are discussed during monthly zoom discussions with the Wannier90 developers.

QUESTAAL: Jerome Jackson was invited to present the Questaal project at the Computer Physics Communications seminar series on July 27 in a talk entitled "Questaal: A package of electronic structure methods based on the linear muffin-tin orbital technique" https://cassyni.com/events/KUusHELFxYN6EJDaB67B5o. A hands-on course (CECAM flagship school) for advanced uses of the code is in preparation for 10-12 May 2022. Testing and maintenance is on-going including a rewrite of the dielectric code. A new version is to be released May 2022.

SPR-KKR: Jerome Jackson and Leon Petit took part in the Ecole de Physique des Houches : "The multiple scattering Green's function approach to electronic structure and spectroscopy calculations", presenting posters on respectively The QUESTAAL code, and magnetism in Gd-intermetallics. The school provided ample opportunities to discuss and collaborate with colleagues, especially with the developers of the SPR-KKR code. The latter is used by the Daresbury team in connection with various projects: Jerome Jackson collaborating with Sheffield Hallam University on the TERASWITCH project, investigating THz driven magnetization switching (paper in preparation), Leon Petit collaborating with colleagues in India on studying the electronic structure of Ru-based Heusler alloys and Ce compounds, as well as collaborating with the Engineering group of SCD on the molten salt project. An SPR-KKR hands-on course at Daresbury laboratory was organized and took place in November 2021.

CRYSTAL: A code freeze was imposed on CRYSTAL in early May to allow extensive for testing of all existing and new functionality for a release of CRYSTAL22 in Q2 2022. Barry Searle gave separate live demonstrations at the MSSC2021 online Crystal school on using DLV to the basic and advanced tutorials. 100 students (65 in basic course, 35 in advanced course) attended.

Other Materials Science related activities: Leon Petit co-authored an article on Hubbard models for optical lattices https://doi.org/10.1103/PhysRevA.104.053321 with colleagues from Open University,

and gave an invited talk online on the Perdew-Zunger-SIC at Conference on Recent Advances in High Pressure Science and Technology in India.

CCPNC

For some of this period the amount of support for CCP-NC dropped down to between 0.3 and 0.5 FTE and so activity, particularly in terms of training and outreach, has been significantly reduced. The main target achieved was hiring a new person to support CCP-NC full time. The new person, Kane Shenton, took up his role part time from July 2021, and switched to full time in October. In addition, work has started on the development of MagresView 2.0, with an initial framework established for a first, basic demo. A beta version, which implements much of the core functionality, is currently being evaluated by users. Work has also gone into developing the theory of dipolar second moments, which has resulted in a script and a paper draft.

The focus of the second half of this period has been on re-building community interactions and support. The CCP-NC's website has been completely refreshed, both in terms of content and presentation, removing outdated entries, adding new information, and restructuring the page for easier navigation. In addition, an online discussion platform, Discourse, has been set up to facilitate interactions between members of the CCP-NC community as well as to serve as a knowledgebase for new users starting out with NMR crystallography. Consultation with various research groups to understand their needs and to better tailor the software and documentation we support has been a priority. Dispersion corrections to density functional theory was one area that was identified needing documentation and Kane has written draft documentation on this for in a new CASTEP documentation website.

Work has also begun on a software renewal project to tackle disorder in molecular crystals, with a rough prototype ready to be tested on realistic examples from the community.

In addition, we have had discussions with other groups within CoSeC and identified several areas of overlap in interest as well as complementarity in knowledge/skill sets. As a result, several joint projects are being planned that will allow us to support our communities more efficiently.

UKCP

In April the annual CASTEP core developers coding workshop (a.k.a. "Codefest") was held virtually. 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. An in-person Codefest has been arranged for April 2022.

The release of academic CASTEP 20.1.1 in March 2021 directed users to the new STFC-run licensing and digital distribution service at https://licenses.stfc.ac.uk. During the reporting period 569 research group licences were issued world-wide. CASTEP licensing for academics has been a successful pilot on the platform, which is available for CoSeC supported projects upon request. Continued maintenance to the Bitbucket code contribution workflow and continuous integration testing on Anvil (https://anvil.softeng-support.ac.uk/) keeps the codebase maintainable and stable.

CASTEP 21.1.1 for academics was released in December 2021 alongside a revised licence application workflow coordinated with Cambridge Enterprise, who own the IP for CASTEP. A revised interface for CASTEP to use the popular libXC library has been developed between Durham, York, and STFC-RAL. CoSeC support coordinated this effort and has been delivered in the CASTEP repository for the version 23 release. Reprioritisation of effort into the libXC and academic licensing changes has moved milestones on the YAMBO interface and van der Waals functional implementation into 2022/23. Work

on the CASTEP 22.1.1 release is complete, except for the port and packaging of the Multi Objective Genetic Algorithm tool. As such, it has been agreed to delay the 22.1.1 release to early Q2 2022.

MCC

ExCALIBUR: Ian Bush, Alin Elena and Tom Keal continue to participate on the steering group of the Materials and Molecular Modelling Exascale Design and Development Working Group (MMM DDWG) under the EPSRC ExCALIBUR programme. The first phase of the project concluded at the end of the July, and as co-Is they have since helped to shape the £2.9m "PAX-HPC" proposal for the next phase. This was successful and is taking forward developments to address the three exascale challenges identified in phase 1 (large scale calculations, complex workflows and I/O), with an emphasis on heterogeneous architectures. They also took leading roles in the community effort to shape the MMM application case studies that are informing these developments, and were co-authors of an article accepted in a special issue of Computers in Science and Engineering detailing these. They organised and participated in meetings with the Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics DDWG which resulted in the two DDWGs identifying commonalities that formed the basis of the combined bid into the next phase, which began in December. A recruitment exercise is now underway for Accelerator Development and Multiscale Workflows PDRA positions funded by the PAX-HPC grant. A PAX-HPC project kick-off meeting was held at Daresbury in March. Ian and Barry have also provided CRYSTAL benchmark cases to the ExCALIBUR exascale challenge problem set.

Benchmarking: After initial problems due to software licensing issues, it was agreed that the effort should focus on classical MD, in particular comparing DL_POLY and LAMMPS. An initial set of test cases have been developed, strongly based upon earlier work by Alin, which examine distinct parts of the forcefield, and again with Alin's help appropriate inputs for the two codes have been written. So far work has focused on a simple Sodium Chloride test case, and it has been shown that the two codes can generate the same scientific results over extended runs. As for benchmarking the situation is complex; using runs that generate the same statistical results LAMMPS evaluates the short-range terms and neighbour list more quickly than DL_POLY, while at least when high accuracy is required DL_POLY has an appreciably faster Ewald sum. The nett result is that at high accuracy DL_POLY is somewhat faster, while when lower accuracy is allowable the situation is less clear, LAMMPS seems to be faster but this is still being evaluated.

CRYSTAL: Barry Searle has compiled and tested the both the current and candidate releases of the code on ARCHER2 and is supporting it for the user base on that machine. Through this, bugs in the software provided on the machine have been uncovered and reported. Ian Bush has started investigating the potential use of ELSI and hence ELPA as a diagonaliser. This is a potential route to the use of GPUs by the code.

ChemShell/DL-FIND: Support of ChemShell development has focussed on enabling use of the Py-ChemShell package on a wider range of HPC platforms, particularly ARCHER2, where efforts to port the code using GNU compilers have now been successful after overcoming a number of issues with the programming environment. An interface to Molpro has been added to enable future excited state and wavefunction-in-DFT developments. Support for the open source version of DL_POLY (DL_POLY 5) as an MM driver has been added, and several interfaces have been updated including LSDalton and NWChem. The 21.0 release was made in December with significantly enhanced functionality and performance. The legacy Tcl-ChemShell and GAMESS-UK packages also continue to be supported and issues addressed as they arise.

DL_POLY/DL_FIELD: The software development on DL_FIELD continued to focus on workflows and improving ease of use. This included reprogramming PDB file interpretation within DL_FIELD to achieve a closer integration with ChemShell for setting up QM/MM models for protein systems. On setting up complex multiple potential systems such as organic-inorganic systems, the auto mixing of van der Waals parameters by using Slater-Kirkwood formalism has been implemented. This would allow users to use atomic information such as atomic polarisabilities to derive the Lennard Jones parameters. Version 4.8 released in September that included the features mentioned above. After moving the DL_POLY package to an open source licencing model, the code has been examined for inconsistencies and ported to ARCHER2. MCC have been assisted with explaining functionality and looking at side effects in applying radiation damage events. The projects were highlighted and training and lectures, targeting ChemShell, were given at the PRACE Autumn School 2021 in Sofia, Bulgaria. Targeted lectures and training, including compilation and performance scaling runs, were also provided in the PRACE Winter School 2022 on the HPC Discoverer part of the Balkans Digital Hub in Sofia.

Biological Science

CCPBioSim

The Enlighten/ChemShell short project has finished. This adds QM/MM functionality to Enlighten (a plugin to the PyMol visualisation software) which is aimed at making simulations accessible to users who are not experienced computational chemists. The new functionality was demonstrated by Sarah Fegan as part of the Enlighten and ChemShell workshops in the CCPBioSim training week.

The TRex short project began in June. A development server has been provisioned within the STFC cloud and the original Rex server deployed. A code review has been completed and tasks assigned to further develop the platform. The first example software programs have been installed.

The short project “Poseidon” to make the code for calculating entropy through the multiscale cell correlation method available to the wider community has started in September. We have reviewed the existing codes from Richard Henchman’s research group and are developing some tests prior to merging the two codes (one designed for proteins and one for solvents). The input parsing functions will need to be rewritten to work with trajectories from recent versions of the MD codes.

Progress on the project to port the FFEA physics is proceeding as planned. Work in this period focussed on deriving the remaining divergence operators required to implement the full FFEA physics in CDO form and implementing the implicit part of the soft body equations. A test case corresponding to the unsteady 1-D heat equation was developed and applied as an analytical solution, in the form of a series; and then used to extend to 3-D in order to solve the vector form of the equation.

The server that the website is hosted on has now been updated to Ubuntu focal (20.04) and the website containers brought up to date with the latest server software utilities. The training platform has been updated to have the kubernetes host servers running on Ubuntu focal, and upgraded to be running the latest kubernetes 1.22 series. Each container has been updated to the latest base container due to a serious root escalation bug, along with this all libraries and packages have been updated for 17/21 training courses we have in our library. The remaining 4 containers are being reviewed to either be updated with the latest ways of working or to be retired as obsolete. Support has been given to authors of courses to establish four new training courses within our catalogue.

The CCPBioSim training week was held online again this year. Participants were able to book sessions individually to suit their interests and schedules. There were an average of 25 people in each session (6 workshops and 2 research seminars). We would like to thank Martyn Winn and Andrea Thorn

(CCP4/CCP-EM) for providing the workshop on Validation of Structures from the PDB. Pietro Faccioli (Universita' degli Studi di Trento) and Denise Okafor (Penn State University) gave very interesting research seminars.

Since April 2021 we have organised 5 Industry Seminars – Jianxin Duan (Schrodinger), Silvia Lovera (UCB BioPharma), Ainoleena Turku (Orion Pharma), Nicolas Foloppe (Vernalis), and Anncharlott V. Berglar (SciVisLab). This series has been well attended with 25-60 people at each one. On 2 March 2022, Elizabeth Bent and Mark Parsons spoke about exascale computing and the ExCALIBUR project.

HECBioSim

In this reporting period a large portion of time has been focused on supporting the community with uptake and access to the national HPC pilot machine ARCHER2 and UK Tier2 JADE2 (Oxford) and Bede.(Durham). Support has been heavily focused on supporting the early access programme to ARCHER2, moving early access phase of JADE2 to production and running a call and supporting early access users on Bede.

There has been a large volume of requests across 3 new machines for support from groups and users when accessing the machines for the first time to achieve performance in production in line with our benchmark guidelines. This is mainly due to users being unfamiliar with the new hardware architectures and our benchmark suite tuned to extract even higher performance than previous in a push to raise the bar. These users were all helped to achieve the required performance that they were expecting. To assist with this going forward, more example submit scripts have been included in our examples on the website. We are also planning a resource to highlight some of the parameters from the documentation of various codes that are the most performance sensitive.

There were two complicated issues that required resolution before the consortium could place users on Bede. There was a problem with GROMACS when running multinode, and a problem stopping plumed from building properly on Bede. The MPI issue required specialist debugging and a workaround was found. The plumed issue was also fixed allowing the full support of the usual codes we offer supported access to under HECBioSim.

Bede is also in the process of updating its operating system from RHEL7 to RHEL8, this has meant that all software has had to be compiled and made available alongside the RHEL7 modules. As the machine moves more towards RHEL8 the RHEL7 versions will be removed. Terms of access for HECBioSim users have been agreed with Durham and a call has been successfully run with users now making production use of Bede.

The benchmarks have been tuned for the new architectures and rerun for ARCHER2, JADE2 and Bede with the same software versions with the figures on the website now updated to reflect the figures for the system under load due to the original figures being obtained with empty systems.

A new resource calculator for applicants to HPC via HECBioSim has been developed. This is based on data from real benchmarking data for AMBER, GROMACS, LAMMPS and NAMD on ARCHER2, JADE2 and Bede. The calculator consists of a containerised backend that will run on our kubernetes infrastructure deployed in the cloud which hosts the data model that is used to forecast HPC time requirements based on parameters known by the scientists; such as system size (atoms) how long they want their simulation (ms) and which code and on which machine. The calculator will then return information on how much system resources are required to run this, thus allowing them to easily calculate compute requirements for RAPs or for other grants. This calculator enables beginner PIs and users or non-traditional consumers of HPC, such as experimentalists, to be able to make these estimates and to begin acquiring access. The calculator will also show the energy consumption

estimates for the given simulations and rationalise it against things that users can relate to their life (eg number of hours the average family home could be powered) The tool is now available on the website.

Work on Longbow2.0 has started. Longbow2.0 will modernise against the latest standards and trends within the Python ecosystem and introduce functionality in line with recent trends in hardware features available. The original Longbow was written many years ago before these ways of working and technologies emerged. Work so far has been focused on restructuring the original functionality into a more modular library format for better use in other projects. Functionality to support ARCHER2 and better support for machines with GPUs has already been added in. Support for passwords and SSH keys with encryption at rest has also been added, meaning that users of Longbow2.0 will be able to use ARCHER2 (or other very secure machines) without having to enter their password repeatedly. Work on Longbow2.0 has also begun to introduce a lightweight GUI and also shift from defaulting to "persistent monitoring" to "fire and forget" mode.

The website server has been updated from Ubuntu 18.04 to Ubuntu 20.04 and the website base container updated from Ubuntu bionic to Ubuntu focal, with the php and mysql versions being brought up to the latest main-line versions. The Joomla framework has been moved onto the 3.10.x series of releases which is the set of releases designed to jump to the new major release line Joomla 4.0 which will form an objective in the next work plan year.

Computational Engineering

UK-COMES

The next planned release of DL_MESO (version 2.8) is currently being prepared (for Q2 2022) after completion of the full implementation of fluid-filled vesicles (e.g. red blood cells) as a major new feature for the LBE code and addition of new interaction types to the DPD code. Improvements have been made to DL_MESO's documentation with a revamped user manual, a technical manual for user-developers wishing to add their own features to the codes and tutorials with practical guides for new and existing users on carrying out mesoscale (DPD and LBE) simulations with DL_MESO. A newly designed graphical user interface (GUI) based on Qt and Python is being written to replace the existing GUI written in Java and make it easier for users to setup and analyse their DL_MESO calculations.

A CCP5 summer project (funded by a CCP5 summer bursary for an undergraduate student) was successfully conducted with Prof. Halim Kusumaatmaja at Durham University. The collaboration led to the integration of a free-energy lattice Boltzmann model into the MPLB code based on the easy-to-understand HiLeMMS interface with training provided by us. Importantly, this collaboration tested the practice of a community-drive model, i.e. a functionality developed by a research community being integrated into a code and released for that community.

CCP-WSI+

WP1: The parMupSiF partitioned FSI framework has been permanently renamed to ParaSiF, efforts to develop this framework exist within the CoSeC support for CCP-WSI+ and through other funding initiatives such as the ARCHER2 eCSE programme and the EU H2020 project SLOWD. The goals of the different projects are similar in that they have components of wave structure interaction in their remit, so this represents a good use of resource given the publicly available nature of the framework. In this reporting period the framework has been further developed in terms of its FSI capabilities, with applications to a number of problems involving deformation of beam-like structures and multiphase liquids. It has been deployed on a number of HPC systems (e.g. ARCHER2, STFC SCARF) and work has

begun to understand how to reduce the complexity of deployment to such environments given its reliance on multiple independent solvers and libraries.

Future development of this framework for CCP-WSI+ will revolve around integrating capabilities from the communities existing OpenFOAM based solvers into the interFSIFoam solver. Initially this will focus on the waveFoam solver which is a development of the basic interFoam solver to include enhanced wave generation techniques. In the future this may also include the other major solver related to CCP-WSI+, qaleFoam, which is also interFoam based. However, this is predicated on work being currently performed by STFC CSE staff under an existing ARCHER2 eCSE grant to explore enhancing the overset mesh based coupling approach within OpenFOAM to allow it to be used as part of a partitioned framework based on a code coupling library.

Work to integrate a ParaFEM finite element solution into ParaSiF is ongoing and involves development of a standalone version of the library-based FEM model developed in the OpenFPCI coupled solution. In the meantime, the existing simple FEM solver already developed within ParaSiF and based on the FEniCS framework remains suitable for many problems specific to the CCP-WSI+ community and is being incrementally developed.

The Multiscale Universal Interface code coupling library is now a core approach within the CCP-WSI+ community (and is the basis for the ParaSiF framework). Significant developments have been made to the library over the reporting period and released to GitHub. The C/Fortran/Python wrappers have all been completely redesigned and are complete and a new top-level CMake build system created for the whole library. As part of a related ExCALIBUR project around code coupling, the parallel performance of the library has been significantly improved, with near-perfect scalability demonstrated on ARCHER2 up to around 1000 nodes.

WP2: In order to improve the parallel performance of the CCP-WSI+ OpenFOAM based solvers, a stand-alone decomposePar tool has been created using ParMETIS. This is generally applicable to a number of codes but specifically implemented in a codebase within the CCP-WSI+ code repository. Within the ESI OpenFOAM variant in the CCP-WSI+ code repository, a new capability for dynamic load balancing through mesh refinement has been added. This is under development but represents the foundations of upcoming improvements to the dynamic load-balancing capability of key solvers within the community. This WP is also currently exploring utilising the ESI OpenFOAM MPI communicator splitting capability without changing the based OpenFOAM source code. A proposed restructure of the CCP-WSI+ code repository to use the latest ESI OpenFOAM to improve both code performance and maintainability has also been done during this period and is currently under review.

WP3: This work package is concentrated on delivering continuous update and improvement to the public-facing aspects of the CCP, such as its website, as well as helping aid in its desire to make data meet the FAIR standard. Over the course of this reporting period, significant inroads have been made to define and implement a new Software Catalogue specific to CCP-WSI+ based on a cutting-edge open-source platform. Over this reporting period, the catalogue has been implemented, customised and sections for software, projects and publications defined. A working prototype has been presented to the working group and a collaborative process used to refine it. The existing CCP-WSI+ website has been maintained and the CCP-WSI+ data store updated and news from the community disseminated.

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 capacity. High order accuracy for spatial discretisation enables CHAPSim the capability to capture

subtle characteristics from turbulence and heat transfer with limited numerical dissipation. The multi-dimensional parallelisation makes CHAPSim use the latest advanced HPC systems (i.e. ARCHER2).

During the reporting period, the 'compact scheme' with an up to 6th order numerical discretisation for spatial interpolation, the first and second derivatives has been implemented into CHAPSim. The compact scheme implemented in CHAPSim2 considered both collocated and staggered grid arrangement at various boundaries conditions. The applied compact scheme has been tested in both serial and parallel mode in Archer2. Test cases of solving first derivative and second derivative of given sinusoidal and polynomial functions validated the applied 2nd, 4th and 6th order of the numerical accuracy in both boundaries and the bulk area of the computational domain. All these developed schemes were well integrated with user-friendly application to solve governing equation.

The library '2DECOMP&FFT' has been selected for pencil-domain decomposition and the FFT solver for the pressure Poison equation. This library was tested with a built-in FFT sub-library and different third party FFT libraries, for instance, FFTW, to validate its functions before implementation. After that, the library '2DECOMP&FFT' have been applied to CHAPSim2. Using this library, we tested CHAPSim2.0 in decomposing computational domain into pencil sub-domain and transposing pencil sub-domain into different directions. The FFT solver in '2DECOMP&FFT' has been used in CHAPSim2.0 to solve a Poisson equation with three-dimensional Fourier Transformation. A Taylor-Green Vortex case was tested to validate the feasibility firstly in a serial mode. The parallel mode of application of this library has been applied to CHAPSim2.0 as well. Case testing and code validations are under progress. A higher-order multiple dimensional parallelised CHAPSim (i.e. CHAPSim 2.0) will be launched this year. CHAPSim2.0 would provide the community with a powerful tool for thermal-hydraulic research on more areas (for instance, to capture subtle features with higher-order schemes) with much more improved parallelisation capability in HPC (e.g. ARCHER2). The development of CHAPSim2.0 is a big step to meet current and evolving scientific challenges and hardware capabilities.

The first try of extending CHAPSim2 to GPU was carried out in CoSeC GPU Hackathon. Potential code development for GPU has been discussed.

During this reporting period, in addition to the code development, research study of heat transfer of liquid metal has also been carried out by numerical simulations of flow of liquid sodium in a Y-junction. Three important thermal hydraulic parameters, i.e. the fluid momentum ratio, the temperature differences of two branches and the inlet Reynolds number, were investigated to study their influence on flow development and the mixing characteristics of the flow in the main tube. It is observed that the momentum ratio plays a key role in the mixing flow development and temperature distribution, while the inlet temperature difference has very limited influence on both flow pattern and wall temperature distribution. The inlet Reynolds number has little influence on flow pattern but it dramatically changes the wall temperature distribution. This study of thermal mixing of liquid metal in one of the most widely used pipe junctions reveals different thermal-mixing patterns and thermal stress development under different thermal hydraulic conditions which would benefit the design of robust pipe junctions and valves, and overall safer piping systems.

CCP-NTH has gone live and been well maintained. https://ccpnth.ac.uk.

UKCTRF

SENGA+ is one of the key DNS codes in the UKCTRF for studying fundamental flows with simplified chemistry. In the first stage, I have spent time studying the code to understand its structure by verifying each term in the Navier-Stokes equations and their implementation. Attention has been particularly paid to the implementation of boundary conditions. The objective of the numerical

boundary condition is to specify the desired physical boundary condition while suppressing spurious acoustic wave reflections at the open boundaries. The version of the NSCBC boundary conditions implemented in SENGA+ was from Poinsot and Lele [1], which assumes the flow is locally one-dimensional and inviscid. This version of NSCBC is inadequate when the muli-directionality of the flow at the boundary is significant.

An extended and comprehensive version of NSCBC has been developed by Yoo et al. [2] and further improved by Lodato [3]. I have studied the improved NSCBC outflow boundary conditions which include transverse and diffusion terms. I expanded their formulation in three Cartesian coordinate directions and implemented them in SENGA+. Efforts have been made to account for the edge and corner effect on the boundary conditions. The spherical flame has been used to examine the effectiveness of the improved NSCBC outflow boundary conditions and the parallel performance of their implementation. The flame can maintain its spherical symmetry when it approaches to the computational boundary.

[1] Poinsot, T.J. and Lele, S.K. 1992, Boundary conditions for direct simulation of compressible viscous flows. J. Comput. Phys.101, 104-139.

[2] Yoo, C.S., Wang, Y. Trouve, A. and Im, I.G., 2005, Characteristic boundary conditions for direct simulations of turbulent counterflow flames. Combustion Theory and Modelling 9,617-646.

[3] Lodato, G., Domingo, P. and Vervisch L., 2008, Three-dimensional boundary conditions for direct and large-eddy simulation of compressible viscous flows. J. Comput. Phys. 227, 5105-5143.

UKTC

In the first half of FY2021-22, we reported that UKTC effort has been greatly reduced due to budget constraints and this has significantly affected the amount of work undertaken. Our intention was for work plans from FY2020-21 to be carried forward into the second half of the year. However, it was decided to reduce the UKTC effort to allow the CCP to be fully supported. A small amount of work was undertaken to scope out how we could integrate particle tracking into Xcompact3d.

CCP Turbulence

The developments of the stfc-branch (https://github.com/rfj82982/Incompact3d) of Xcompact3 have been merged into the Master branch, and a few scalability tests are still necessary to assess that the scalability of the code on ARCHER2. This includes a new installation and testing based on CMake/CTest, a reorganisation of some core subroutines of the code (i.e. the Poisson solver, matrix refinements for stretching in the wall normal direction, adding of new turbulent initialization, etc) and a consistent approach to floating point precision. This work was mainly carried out in the first half of the year.

The second part of the year was dedicated to porting the code to hybrid architectures with a particular focus on multi GPU(s) porting. This work had been carried out on a mini-app called X3div (https://github.com/xcompact3d/x3div), which has all the main features of Xcompact3d (high order finite difference compact schemes, FFT solver for the Poisson equation, pressure correction, etc). A first full implementation with multi-GPU offloading is now available which is based on: managed memory management, automatic optimisation of parallel loop using Fortran parallel paradigms, CUDA aware MPI or Nvidia Collective Communication Library (NCCL) and CUDA FFT for the Poisson solver. A second implementation, exclusively based on openACC, is also available for fine tuning of the optimisation parameters. This version will be mainly useful for cases with large memory requirements.

In the first part of the year, a new documentation framework for OPS has also been created, which facilitates the concept of continuous integration. Once developers update the explanation on functionalities in an easy-to-use markdown format, the “new” documentation will be automatically

generated and shown at https://ops-dsl.readthedocs.io. The previous one in a latex file is being transformed to the new system. Moreover, the Gitflow workflow is being promoted for version management.

In the second part of year, new applications are added into the OPS for demonstrating the usage of tridiagonal linear solver for solving the Burgers equations and implementing the high-order compact finite difference scheme.

Tomographic Imaging

CCPi

In the reporting period we have published 2 articles on the Core Imaging Library (CIL) appeared on the Royal Transaction A in July 2021, documenting the capability of the software and providing use cases. The team has contributed to the submission and review of 2 other articles using CIL, one published in Journal of Physics D: Applied Physics and one in Nature Scientific Reports.

CCPi has engaged with users at a number of conferences in the reporting period. Both talks and posters were presented at iBSim and ToScA, and a talk was given at the Manchester ideas forum.

There have been 3 releases of the CIL software published in this period adding functionality and addressing issues on the code, versions 21.1.0 and 21.2.0., 21.3.1.

On May 26th a one-day online workshop on Digital Volume Correlation (DVC) was organised in collaboration with the University of Portsmouth and was attended by 80 people worldwide. The CCPi solution has been presented by Prof. Brian Bay and a network mailing list for DVC was launched.

The first prize in the CoSeC Impact Award 2021 has been awarded to Ryan Warr from University of Manchester, for his work supported by CCPi: SCD Winners of the 2021 CoSeC Impact Award (stfc.ac.uk).

The CoSeC team has supported and continues to support large facilities such as ISIS/IMAT, CLF/EPAC and external partners such as QMUL, UCL with bespoke software based on CIL for their beamlines. In particular the collaboration with QMUL has brought the development of the optimised Filter Back Projection algorithm.

CCPSyneRBI

Our work during the reported period mostly progressed according to the job plan with adjustments to avoid face-to-face meetings. We continued our software development and engineering efforts, adding content to our website www.ccpsynerbi.ac.uk, maintaining our steadily growing mailing lists (we now have 103 members on the announcement list, 38 on the developers and 82 on the users' lists), organising online meetings, training courses and Hackathons.

A large amount of work went into preparation and running of an online training course (see "training" section below).

On 20 May 2021 we released SIRF 3.0, on 24 June 2021 SIRF 3.1 and on 6 July 2021 SIRF 3.1.1. In these versions of SIRF, we updated versions of software packages on which SIRF depends and incorporated new functionality, with as highlight preliminary support for the PET data of the GE Signa PET/MR scanner and additional GPU projectors for PET. These releases also contain contributions from the community (merged with assistance from CoSeC) and in particular the support for our first non-Cartesian MR sequence. Finally, we also transitioned our Continuous Integration (CI) testing to GitHub Actions instead of previously used Travis CI due to continuing problems with credits on Travis CI.

On 17 Sep 2021, we held the third Steering Panel meeting of CCP SyneRBI, on which we reviewed the progress in the implementation of the 3 Work Packages of our Project Work Plan: 1) Networking activities and Community Engagement, 2) Research software development, and 3) Translation towards Biomedical researchers, and discussed further steps to be taken.

Our 8th Hackathon took place on 23 to 26 Nov 2021, with face-to-face sessions in Cosener's House, Abingdon, on 23 and 24 Nov followed by online sessions on 25 and 26 Nov. The goal of this hackathon was to establish a benchmark between the numerous iterative algorithms for CT and PET reconstructions that have been proposed in the recent years, with a focus on randomized algorithms. There also was a group working on subset data structures in STIR to enable efficient computation on subsets of scanner data.

The latest version 3.2.0 of SIRF was released on 22 March 2022. It is the first SIRF version that is capable of handling non-cartesian MR encoding trajectories: 2D radial, golden-angle increment radial and stack-of-stars, and exposes advanced parameters from STIR RayTracingMatrix object to SIRF C++ and Python interfaces.

Atomic and Molecular Physics / Plasma Physics

HEC Plasma

Unfortunately, direct CoSeC support for HEC-Plasma was ended in 2021-2022, owing to CoSeC budget cuts and non-availability of staff to take over work from Dr Joseph Parker (now at CCFE). The main highlight of the year was the (13-15 April 2021) joint UK-AMOR (and CCPQ) – CCP/HEC-PLASMA workshop, 'Atomic and Molecular Data Needs for Plasma Applications', with ~160 registered participants, 23 talks, 3 informal discussion sessions, a demonstration by Quantemol Ltd and a poster session. The posters and talks are preserved on the CCPQ website (and a summary proceedings documented is planned to be made available).

In addition, Joseph Parker has published a paper in the Journal of Computational and Applied Mathematics on his developmental work while in SCD.

UK-AMOR

With limited support and no longer any back-up CCPQ support, activities this year have concentrated on new funding opportunities. However an early highlight (13-15 April 2021) was the joint UK-AMOR (and CCPQ) – CCP/HEC-PLASMA workshop, 'Atomic and Molecular Data Needs for Plasma Applications', with ~160 registered participants, 23 talks, 3 informal discussion sessions, a demonstration by Quantemol Ltd and a poster session. The posters and talks are preserved on the CCPQ website. Martin Plummer applied and secured STFC Ada Lovelace Centre funding for a 6-month placement for an STFC Graduate Employee to work on the UK-AMOR RmatReact theory (and code), September 2021 to March 2022, in preparation for introducing rearrangement channels (reactions) into the package. Martin Plummer has also worked with PI MM Law (Aberdeen) on a proposal to adapt and use RmatReact for low-energy antimatter, specifically anti-H collisions with molecular hydrogen of direct relevance to the CERN ALPHA project (co-I Martin Plummer, project partners J Tennyson and M Charlton (Swansea and ALPHA)). This proposal is now ready to be submitted in June 2022. The Graduate project (supervised by Martin Plummer) has been a great success and informed the proposal, investigating the combination of mixed and single-system Jacobi-like coordinates needed for rearrangement R-matrix collisions: the future application of the work to CERN experiments was the main reason the Graduate project was funded. [Martin's main scientific coding has been on UK-AMOR's RMT code, part of the eCSE project and EPSRC AQuA-DIP grant obtained in 2020-2021.]

Martin also contributed to UK-AMOR's submission to EPSRC's Research for Software Communities Call, 'Data standardisation and Interoperability for Novel AMO Research (DINAMO)', PI Dr JD Gorfinkiel (OU). UK-AMOR member Dr D Green (Queen's University Belfast) was awarded an Access to HPC ARCHER2 award (Martin assisted with the Technical Assessment for the antimatter code ANTI-ATOM). CoSeC central office support managed the registration page for the forthcoming ATTO-FEL 2022 workshop (UCL, 27-30 June 2022) for Attosecond and Free Electron Laser Science. In addition, further work has been done on the UK-AMOR PFARM code by Andrew Sunderland as part of a separate PRACE project, both in preparation for energy efficiency adaptation and as part of a new release of the Unified European Applications Benchmark Suite (both CPU and GPU), which would not have been possible without the earlier CCPQ/UK-AMOR support work.

Quantum Computing

CCP-QC

Working group two (Martyn Winn, Ronan Keagan, Andrei Lebedev, Ville Uski, Alin Elena, STFC, Nicholas Chancelor, Viv Kendon Durham, Animesh Data, Warwick and Adam Callison UCL) meets regularly working on quantum algorithms for crystallographic problems mainly phase estimation. Majority of the meetings are online due to covid but we have managed a first face to face meeting at RAL in September.

Alin Elena was part of the organising committee of the Integrating Quantum Computers in Condensed Matter Physics Simulations, National Physical Laboratory, 23rd-24th September 2021 with invited speakers Professor Viv Kendon, University of Durham, Dr Tom O'Brien, Google, Professor Emanuel Gull, University of Michigan, Dr Panagiotis Barkoutsos, IBM Europe, Zurich, Professor Mónica Benito, University of Augsburg, Germany, Dr Ash Vadgama, National Quantum Computing Centre. The event was hybrid with 120 attendees online and 25 in person in NPL. A follow up workshop will happen next year in Manchester at European Physics Society conference.

Alin was also invited at the ground breaking ceremony at the National Quantum Computing Centre site at Rutherford Appleton Laboratory.

Working group 2 Crystallography and Quantum Mechanics was part of the CIUK 2021 CoSeC workshop where progress was presented. WG2 will hold a community workshop to showcase the outcomes of the work in Q2 2022, most probably in London.

Working group 3 was set-up, with Dominik Joachim doing the work, concentrating on quantum computing and electronic structure.

At the European Physics Society and Institute of Physics conference, AME will be part of the organising committee of the mini-colloquium Integrating Quantum Computers in Condensed Matter Physics Simulations, August 21-26 2022 https://iop.eventsair.com/cmd29/integrating-quantum-computers-in-condensed-matter-physics-simulations.

Underpinning Technologies

Software Outlook

Software Outlook's latest best practice guidance report has been released, focussing on software testing (https://www.softwareoutlook.ac.uk/?q=bestpractice). This guidance will allow CoSeC Developers to focus their software testing efforts in the manner most suited to their projects and available resourcing: to ensure that the software is reliable and serves its purpose, it is important that a structured testing strategy is used.

As part of the CoSeC Working Group on Code Coupling, Philippa Rubin gave a seminar on the Software Outlook Code Coupling work, which was well received (a recording is available via https://www.softwareoutlook.ac.uk/?q=code_coupling). She has completed the accompanying report, which is also available via Software Outlook's Code Coupling webpage.

We also released our technical report summarising the different frameworks available for exploiting hybrid (CPU+GPU) architectures and comparing them (https://www.softwareoutlook.ac.uk/?q=hybridgpu).

Appendix - Individual CCP/HEC Work Plan Updates 2021-22

This appendix contains updates on the full, individual work plans for 2021-22 for the CoSeC supported CCPs and HECs. Tasks highlighted yellow indicate a change from the plans submitted in the 2020-21 annual report, 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
	Respond to recommendations from the SLA Review 2018	Ongoing
	Weekly internal STFC meeting to discuss progress with all CoSeC activities	Ongoing
	Arrange internal project meetings with funded CCPs and HECs – April 2020 – individual meetings Complete	Q2 2021
	Prepare and submit CoSeC annual report – June 2020 Complete	Q2 2021
	Arrange and attend the CCP Steering Panel May meeting Complete	Q2 2021
	Attend the CoSeC SLA Steering Committee June meeting Complete	Q2 2021
	Arrange internal project meetings with funded CCPs and HECs – July 2020 – DL / RAL site meetings Complete	Q3 2021
	Compile and submit ARCHER renewal proposal Complete (Martin Plummer)	Q3 2021
	Arrange internal project meetings with funded CCPs and HECs – October 2020 – individual meetings Complete	Q4 2021
	Prepare and submit interim CoSeC SLA report – November 2020 Complete	Q4 2021
	Arrange and attend the CCP Steering Panel December meeting Complete	Q4 2021
	Attend the CoSeC SLA Steering Committee December meeting	Q4 2021

	Complete	
	Arrange internal project meetings with funded CCPs and HECs – January 2021 – DL / RAL site meetings Complete	Q1 2022
Impact	Carry out outreach activities (social media, brochures, talks)	Ongoing
	Maintain and update CoSeC web site	Ongoing
	Write and publish CoSeC news articles on the CoSeC website	Ongoing
	Facilitate CCP/HEC website re-design	Ongoing
	Administrate CoSeC Impact Award Complete	Q2 2021 – Q1 2022
	Design CoSeC branded (and environmentally sustainable) publicity and outreach material for workshop/conference handouts	Q2 2021 – Q4 2021
	Write and publish CoSeC Impact Award 2021 case studies Complete	Q3 2021 – Q4 2021
	Launch the CoSeC Impact Award 2022 Complete	Q4 2021
Technical	Continue to grow thematic working group process (new groups, continuation of existing and tangible outputs)	Ongoing
	Define continued (annual) activity based on initial 2021 meeting	Ongoing
	Scope and create internal CoSeC skill-sharing exercises	Ongoing
	Begin and solidify thematic working group process within CoSeC Ongoing	Q1 2021
	Scope and define initial annual CoSeC meeting/conference concept for 2021 Complete	Q2 2021
	Organise and facilitate initial CoSeC meeting for 2021 Complete	Q4 2021
	Explore formalised CoSeC-specific scientific output (i.e. curation of a journal special edition or a specific CoSeC publication) – linked to annual meeting concept Ongoing	Q4 2021

Materials Science

CCP9	Milestone	Target Date
	Link QUESTAAL's lmf to SPEX code Ongoing	~~Q2 2021~~ Q4 2022
	Submit paper on incommensurate ordering in CrB2 Complete, awaiting submission	~~Q2 2021~~ Q2 2022
	Tutoring at CRYSTAL school Complete	Q3 2021
	Publish paper on programmable potentials in optical lattice Complete	Q3 2021
	Wannier90 Library, make parallel and thread safe (phase 2) Complete	Q3 2021
	Widening participation workshop with SuperSTEM Postponed, possibly Q3 2022	Q3 2021
	Organize KKR workshop Complete	Q4 2021
	BSE spin susceptibilities implemented in QUESTAAL (phase 2) Ongoing	Q1 2022
	Organize QUESTAAL school Complete, scheduled for May 2022	~~Q4 2021~~ Q2 2022
	Wannier90 Library postW90 extension Ongoing	~~Q1 2022~~ Q3 2022
	Testing CRYSTAL22 release candidate Complete	Q1 2022
	CRYSTAL parallelization extended to CPKS equations Target contingent on Crystal 2022 release	~~Q1 2022~~ Q4 2022
	DMFT verification QUESTAAL/CASTEP (preparation phase) Delayed	~~Q1 2022~~ Q1 2023

CCPNC	Milestone	Target Date
	Maintenance and further development of Soprano	Ongoing
	Maintenance and further development of CCP-NC database	Ongoing
	Full integration of MagresPython and Soprano, and development of documentation and tutorials to ease the transition, in consultation with users.	Ongoing

	Finish development of MagresView 2.0, deploy and test Completed majority of core functionality, though user feedback suggests there is still further work needed before a full release.	Q1 2022
	Example application of the new CASTEP NEB implementation to NMR in disordered or dynamical systems Completed, with more examples to follow.	Q1 2022
	Engagement with users to develop outreach, provide material for website, guide priorities for CCP-NC tools (especially programmatic tools for NMR crystallography), and develop user engagement strategy. Complete	Q1 2022

UKCP	Milestone	Target Date
	Maintenance of CASTEP user licensing and source code distribution.	Ongoing
	Maintenance of CASTEP code repository and continuous integration system.	Ongoing
	Release management of CASTEP v21 including documentation and liaison with major HPC services.	Q2 2021
	Support release of Genetic Algorithm tool to coincide with academic CASTEP v21.	Q2 2021
	Launch of ORCiD-authenticated CASTEP download web page.	Q2 2021
	Produce interface for CASTEP to YAMBO.	Q3 2021
	Co-organization and teaching of CASTEP workshop(s).	Q3 2021
	Organisation of 2022 CASTEP "codefest" core developer workshop.	Q4 2021
	Prototype implementation of van der Waals DFT (Dion) functional in CASTEP.	Q4 2021
	Release management of CASTEP v22 including documentation and liaison with major HPC services.	Q1 2022

MCC	Milestone	Target Date
ExCALIBUR	Attend MMM DDWG steering group meetings and help organise monthly meetings of the full DDWG Meetings were held throughout this period, including community discussions to identify key application case studies, and regular	Q2 2021

	steering group meetings continued in preparation for the funded phase 1b extension	
	Blueprints for “hero calculations”, complex workflows and I/O A set of blueprints for phase 2 were drafted under each of these themes informed by the scientific application case studies, and work began on the identified developments in Q4 (partially supported by MCC), with two recruitments to work on Accelerator Development and Multiscale Workflows to follow.	Q2 2021
	Setup MOF inputs in aiida for I/O bechnmark The setup of MOF workflow is done via aiida and cp2k. A suitable system for the task need to be identified. Calculations requires 4000 nodes so probably only ARCHER2 can provide that in UK	~~Q2 2021~~ Q1 2022
	Get access to one of the storage prototypes and benchmark hdf5 io from lammps Access to the IO testbed has been secured, benchmarking to be done	~~Q2 2021~~ Q1 2022
Benchmarking	Identify with the community the classes of codes used *Ab initio* DFT electronic structure and classical MD codes were identified	Q3 2021
	For at least 1 of those classes identify appropriate scientific problem(s) within the community that are being solved A set of problems for the classical MD codes DL_POLY and LAMMPS have been identified that stress different parts of the forcefield	Q3 2021
	Demonstrate obtaining the same answer to the problem(s) with more than 1 code in the class – or report why differences occur. An Initial demonstration has been performed for a NaCl test case	Q1 2022
	Benchmark the codes on architectures of interest and provide a report on the results. Initial results suggest for high accuracy simulation DL_POLY is faster on Archer2 than LAMMPS, but the situation *may* be reversed for less strict tolerances	Q1 2022
	Supporting relevant code developments ELSI is being investigated in CRYSTAL	Ongoing
ChemShell/ DL-FIND	Interface to Molpro Work complete (Task carried over from 2020/21 due to delay in licencing Molpro)	Q3 2021
	~~Improved set of materials modelling tutorials~~ Deprioritised in favour of Molpro interface work as prerequisite code improvements have not yet been received. Task will be rescheduled when these improvements are in place.	~~Q3 2021~~
	New release of Py-ChemShell The 21.0 release was made available in December with a further update (21.0.1) in February following a code review including	~~Q3 2021~~ Q4 2021

	additional bug fixes, HPC platform enhancements, documentation and tutorials.	
	Implement a framework for multiple electronic state QM/MM calculations and interface to DL-FIND for conical intersection optimisations. Excited state calculations are available via QM code interfaces. Full framework delayed to prioritise an additional full code review leading to version 21.0.1 and extensive optimization work on the new full ARCHER2 system.	Q1 2022
	Port, optimise and maintain ChemShell on ARCHER2 and Tier 2 systems (e.g. YOUNG) Both Tcl-ChemShell and Py-ChemShell have been successfully ported to ARCHER2 using GNU compilers and now being prepared as centrally installed modules on the full system. Both codes are also available and maintained on YOUNG.	Ongoing
DL_POLY	Port, optimise and maintain DL_POLY_4 on ARCHER2 and Tier 2 systems and support user community on-line. ARCHER2 port is done. A number of compiler flagged bugfixes are tackled.	Ongoing
	Investigate performance and scalability of short-range forces evaluations in DL_POLY_4. Complete based on tests by Alin Elena (MMM DDWG) and discussions with Ian Bush it is unclear what part of the two body procedures is the bottleneck. Further investigation is needed.	~~Q3 2021~~ Q3 2022
	Re-engineer the frozen-frozen coulombic interactions exclusion routine to be exact for large systems (and avoid discrepancies between virial and energy due to an implementation that approximates the interactions due to memory requirements). Now targeting Q4 2022 for this task as no DL_POLY effort will be booked in 2022.	~~Q4 2021~~ Q4 2022
DL_FIELD	Improve automation of organic-inorganic non-bonded interactions - Continuation No MCC project effort was booked during Q1 2022. This work effort is postponed till 2022/23 (See below).	~~Q4 2021~~ Q4 2022
	Enable solvation in multiple potential settings and for all types of system models, including bio-inorganic models - Currently, solvation features only work for organic systems in a single-potential scheme setting, on organic system models. Completed. Users can now specify solvents from any available FF schemes.	Q1 2022
	Software release, version 4.8 - Released in September 2021 as planned (Q3 2021). Version 4.81 was released in Q1 2022, mainly to improve program stability, and remove memory leaks issue especially for multiple potential settings.	~~Q3 2021~~ Q1 2022

Biological Science

CCPBioSim	Milestone	Target Date
	Add modules to the online training and lead/support workshops New training has been added – Introduction to Reduce and Propka, Introduction to Clustering, and Introduction to DNA Simulations.	Ongoing
	Maintain CCPBioSim portfolio of codes on Github.	Ongoing
	Maintain and develop cloud infrastructure for CCPBioSim website and training programme. The cloud infrastructure has been successfully used for the CCP5 Summer School and the CCPBioSim Training Week	Ongoing
	Wrap up 2021 multiscale modelling conference and consult on plans for the future of the conference series The 2021 Multiscale Modelling Conference was a success, the first of the series to be held online.	Q2 2021
	CCP short project #1. Finish Enlighten/ChemShell project and plan for Enlighten/ChemShell workshop using case study A demo of the new functionality was part of the CCPBioSim Training Week.	Q2 2021
	CCP short project #2. TRex (Tool for Remote Execution) – a software as a service project. June - August 2021, Dec 2021 – Feb 2022 Development server provisioned within the STFC cloud and code review completed. Propka and WaterDock2.0 have been installed on the server.	Q4 2021
	Validation of the new FFEA framework in Code_Saturne, and testing at scale, with the objective to run test simulations up to the whole ARCHER2. Work ongoing to derive full framework	Q1 2022
	CCP short project #3. Poseidon – a new tool for calculating entropy. Sept – Nov 2021, Mar – May 2022. Recently started work on this project.	Q2 2022

HECBioSim	Milestone	Target Date
	Maintain cloud based web and training infrastructure	Ongoing
	Maintain HECBioSim webserver and website	Ongoing
	Maintain the HECBioSim benchmarks with regular tests on new software releases across T1 and T2 HPC	Ongoing

	Support the consortium users of HPC with ARCHER2, JADE, JADE2 and Bede with performance issues, software issues, running issues, questions on how much resource etc.	Ongoing
	Develop and release new HPC calculator for the new ARCHER2 and Tier2 HPC machines Complete	Q2 2021
	Benchmark Tier2 Wilkes3 that is part of CSD3 and write up the benchmarks on the website Delayed initially due to machine deliver delays. Delayed to following reporting year due to redeployment of staff	Q2 2021 TBC
	Longbow v2021.0 Delayed due to following year due to redeployment of staff.	Q1 2022
	TBC – Exascale version of FFEA – under project scoping Scoping exercise completed, a grant application is currently being submitted to take this work further as it is too much work for the resource available here.	Q3 2021

Computational Engineering

UK-COMES	Milestone	Target Date
	Release a new version of DL_MESO (2.8) Delayed due to completing fluid-filled vesicle implementation, but on target for new due date.	~~Q2 2021~~ Q2 2022
	Improving the stream-collision scheme in MPLB to optimise memory usage Completed after final comparison and integration postponed to Q1 2022.	~~Q3 2021~~ Q1 2022
	Inclusion of LBE suspended particle models in DL_MESO Due to start after release of new version of DL_MESO: target date postponed accordingly.	~~Q4 2021~~ Q3 2022
	Release a new version of MPLB code Complete. Gitflow workflow on Github implemented to continuously merge new features into the development branch prior to future releases.	Q1 2022

CCP-WSI+	Milestone	Target Date
	Detailed technical report of dynamic load balancing implementation within ESI OpenFOAM port. Complete	Q2 2021

	Software Catalogue framework implemented, demonstrated and agreed. Complete	Q3 2021
	Code Repository Development and maintenance. Progressing well. Activity has proven more complex so new tasks taken into 22/23 plan.	~~Q1 2022~~
	Implementation of standardised CCP-WSI+ PoC coupled framework for WSI (~~parMupSiF~~ ParaSiF framework key output – new tasks relating to this created). Complete	Q3 2021
	Create stand-alone solver using ParaFEM, based on OpenFPCI solution. Delayed due to effort availability within Manchester.	~~Q1 2022~~
	Final report on wsiFoam performance benchmarking and optimisation. Delayed due to unforeseen staff circumstances.	~~Q3 2021~~ ~~Q1 2022~~
	Implement new dynamic load balancing library for ESI OpenFOAM. Complete	Q4 2021

CCP NTH	Milestone	Target Date
	CHAPSim2: to develop and test 'compact scheme' for CHAPSim2.0 in various conditions in Archer2 Completed.	Q4 2021
	CHAPSim2: to develop and test the Poisson solver for CHAPSim2.0 Ongoing.	Q1 2022

UKCTRF	Milestone	Target Date
	Understand and set up a test case for SENGA+	Q2 2021
	Understand and examine available NSCBC outflow boundary conditions for SENGA+	Q3 2021
	Derive and implement comprehensive NSCBC outflow boundary conditions including transverse terms in SENGA+	Q4 2021
	Implement diffusion terms in the outflow boundary condition in SENGA+ and set up a spherical flame test case.	Q1-Q4 2022

UKTC	Milestone	Target Date
	Introduce kinetic boundary wall-boundary condition into OpenSBLI	Q3 2021
	Investigate and extend in situ visualisation studies using nek5000	Q4 2021

CCP Turbulence	Milestone	Target Date
	Porting on GPU of XCompact3D by using OpenACC Full porting of the mini-app to multi-GPUs is completed. Two versions are available one which combines parallel features from the native languare (i.e. fortran do concurrent) and openACC and a second with pure openACC	~~Q2-Q3 2021~~ Q1 2022
	Merge of all new features in the main code repository on Github Completed	~~Q2 2021~~ Q4 2021
	Organise a dedicated hackathon dedicated to turbulence community in the UK Completed	Q4 2021
	Develop the Python translator for creating implicit solvers based on OpenSBLI Ongoing. After an initial study on the complexity where significant changes are needed, we extend the task to Q2 2022.	~~Q4 2021~~ Q2 2022
	Explore the porting to Python3 for the OpenSBLI code Canceled	Q4 2021
	Multi-GPUs porting of the code mini-app Completed	Q1 2022
	Start to implement penta-diagonal solver for the OPS code To be started after the development of OpenSBLI work	~~Q1 2022~~ Q1 2023

Tomographic Imaging

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives	Ongoing
	Organise exec 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

	Progressing well. 3 training sessions have been organised, contributing to proposal to EPSRC software for research communities call	
	Embed lab-based framework: UoM/ UoS/ UoW Progressing well: deployment at QMUL and in contact with UCL	Ongoing
	Code integration with CCPPETMR Progressing well.	Ongoing
	CIL as Savu Plugin On hold due to missing support from DLS and low priority	Q2 2021
	Collaboration: Working with Brian Bay (USA) on improving and enhancing the digital volume correlation code Progressing well, added strain calculation to the DVC code, added some multithreading to core code.	Q2 2021
	Release of the digital volume correlation code and distributing it to CCPi community. Q3 2021 DVC GUI and DVC code are distributed for Linux, Windows and MacOSX as binaries. Code not yet licensed.	Q2 2021
	Using the CILViewer for analysis and pre-processing of the data Ongoing work in collaboration with CLF/EPAC	Q2 2021
	Enable remote analysis of tomographic data Low priority, on hold. Parts of the code to achieve this have been developed	Q2 2021
	Publication of a scientific article based on work enabled by CCPi Digital Volume Correlation Ongoing in collaboration with University of Oregon	Q2 2021
	Providing support for iterative reconstruction at facilities ISIS/IMAT On target, a first algorithm has been deployed at IMAT via Mantid Imaging	Q3 2021
	Help to organise the main ToScA conference; September 2021 On target	Q3 2021
	Investigation of ML/AI methods for tomography On hold, low priority	Q3 2021
	Providing support for iterative reconstruction at facilities: DLS i14 beamline: Laminography On hold, missing support from DLS	Q1 2022
	Providing support for iterative reconstruction at facilities CLF/EPAC Ongoing, progressing well, GUI being developed and initial version shown to scientists	Q1 2022

	Analysis of Cryo EM data for COVID-19 On hold. Initial data have been processed but currently missing support from partners.	Q1 2022
	Organise hackathon for development of novel reconstruction algorithms and benchmarking On target	Q4 2021

CCPSyneRBI	Milestone	Target Date
	Complete transition to Python3 on docker, VM and Azure Completed	Q2 2021
	Alternative for Travis.com (Continuous Integrating) Completed (now using GitHub Actions CI).	Q2 2021
	Merge of scripts for VM (via vagrant) and Docker. Near completion	~~Q2 2021~~ Q2 2022
	Further additions to C++ Interface. Ongoing.	~~Q2 2021~~ Q1 2022
	Functions to compute gradients and values of MR objective function. Postponed. Might be dropped in future.	~~Q2 2021~~ Q1 2023
	Run-time optimisation, e.g. by creating subsets of acquisition and image data or multi-threading. Ongoing.	~~Q2 2021~~ Q1 2022
	Sample pipelines for PET and MR reconstruction for static data. Postponed due to 10% reduction in planned CoSeC effort.	~~Q2 2021~~ Q4 2022
	SPECT support including multi-energy window SPECT. Ongoing. Static PET nearly completed.	~~Q3 2021~~ Q1 2022
	MR iterative reconstruction via CIL. Completed	Q3 2021
	Implementation of a few generic optimisation algorithms (with CIL). Completed, although more will be added	Q3 2021
	Tools for working with subsets of acquisition and image data. Ongoing.	~~Q4 2021~~ Q1 2022
	SIRF ~~Release 4.0~~ Release 3.2 Completed, version major left at 3 since no backward incompatibility has been introduced	~~Q4 2021~~ Q1 2022
	Investigate integration of other reconstruction packages. Postponed.	~~Q1 2022~~ Q4 2023

	Investigate installers with precompiled software (conda). Ongoing.	~~Q1 2022~~ Q3 2022

Atomic and Molecular Physics / Plasma Physics

HEC Plasma	Milestone	Target Date
	Workshop 'Atomic and Molecular Data Needs for Plasma Applications' (joint with UK-AMOR and CCPQ) to take place in April 2021, any immediate follow-up to be decided by MP with Ben Dudson and Colin Roach Workshop complete, follow up ongoing.	Q2 2021
	Further follow-up and additional work to depend on effort availability This may be carried out in 2022-2023 under the UK-AMOR remit if resources allow.	2022-2023

UK-AMOR	Milestone	Target Date
	Attend UK-AMOR management committee meetings as required and follow up accordingly. Support workshop organization as appropriate. Atomic Data Needs Workshop complete. CoSeC central office support managed the registration page for the forthcoming ATTO-FEL 2022 workshop (UCL, 27-30 June 2022) for Attosecond and Free Electron Laser Science. A management meeting decided that Professor Hugo van der Hart (QUB) will lead the next UK-AMOR HEC bid.	All year
	Continued work on the bound states code and/or any further follow-up on Eryn Spinlove's work, ideally with practical calculations resulting from this (with strictly limited UK-AMOR support time in 2021-2022, more specific milestones will be held back until after the UK-AMOR management meeting in April and follow-up). Martin Plummer's main scientific/coding work in this period was for the RMT eCSE and the AQuA-DIP project, however the new graduate project has made important progress in examining changes needed to RmatReact to allow rearrangement collisions and introducing coding in mixed coordinate systems. The antimatter proposal (see below) will involve substantial work on RmatReact. Further/major work will be agreed for 2022-2023 as part of the new proposal.	All year
	Look out for new sources of funding to support UK-AMOR core support. STFC Graduate project (6 months September-March, funded by Ada Lovelace Centre) OBTAINED and COMPLETED	All year

	New grant proposal on antimatter work with PI MM Law (Aberdeen) and Martin Plummer as co-I underway now to be submitted in June 2022 (Jonathan Tennyson and Prof M Charlton, Swansea, are project partners). Martin was co-I on the UK-AMOR proposal for the EPSRC Software for Research Communities Call, submitted by 14 October 2021. Unfortunately this was not successful, however the focus on data portability will feed into the HEC renewal. Martin is currently in discussions with Dr D Green (QUB) over possible short term funding (<= 1 month) for work on his ANTI-ATOM code and Martin will also take full part in the UK-AMOR renewal.	
	Check on Andrew Sunderland's finalizing of the parallel UKRMol+ memory optimization extension (assuming the COVID situation becomes more normal) Owing to a domestic emergency, Andy had to take time off for family care. This work is postponed until Andy is available.	Q2-Q3 2021 (now 2022-23 depending on Andy Sunderland's situation)
	Keep track of Andrew Sunderland's PRACE work with PFARM, look for opportunities to extend this: for example examine the possibilities for this work to include to comparison tests with UK-AMOR code PSTGF. Andy has started porting PFARM to the current range of PRACE Tier-0 architectures (CPUs/GPUs) (to progress in earnest by beginning of November). Energy usage monitoring will be a much more significant factor in these benchmark results. The benchmark framework (documentation, run setup scripts and job submission setup scripts) for CPU and GPU runs has recently been developed for the latest release of the UEABS and this has been independently tested by two research groups in Barcelona and Ankara. https://repository.prace-ri.eu/git/UEABS/ueabs. Benchmarks data sets that are more likely to scale up to 100,000 cores. UPDATE April 2022: Recent development work has involved dealing with multiple energy meshes efficiently, creating larger datasets for testing and developing documentation and scripts to automate the setup of parallel runs on a range of CPU and GPU-enabled HPC platforms. PRACE collaborators in Bilkent University and Barcelona Supercomputing Centre completed a formal cross-review of the PFARM benchmark. A recent benchmarking exercise ran the PFARM benchmark on eight Tier-0 systems across Europe. The results and performance analysis were reported in the PRACE 6iP Deliverable D7.4 'Evaulation of Benchmark Performance'. Both time-related efficiency and energy-related efficiency of the large-scale parallel runs were analysed. Performance on the Juwels-Booster Nvidia A100-based system at Forschungszentrum Juelich was particularly impressive, reflecting some of the improvements to the architectural design for dense-linear algebra operations on the latest GPU devices.	Up till Q4 2021

Quantum Computing

CCP-QC	Milestone	Target Date
	Executive committee Complete	Q2 2021
	Executive committee Complete	~~Q3 2021~~ Q4 2021
	NPL workshop Complete	Q3 2021
	Executive committee Ongoing	~~Q1 2022~~ Q2 2022
	Crystallograpy working group (*Note: this milestone is included for information despite falling outside the reporting period*)	Q3 2022
	EPS workshop (*Note: this milestone is included for information despite falling outside the reporting period*)	Q3 2022

Appendix - Individual CCP/HEC Work Plans 2022-23

This appendix contains the full, individual work plans for 2022-23 for the CoSeC supported CCPs and HECs. Tasks highlighted yellow indicate a change from the plans submitted in the interim report, November 2021, 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
	Arrange internal project meetings with funded CCPs and HECs – April 2022 – meetings arranged by scientific field	Q2 2022
	Prepare and submit CoSeC annual report – June 2022	Q2 2022
	Arrange and attend the CCP Steering Panel May meeting	Q2 2022
	Attend the CoSeC SLA Steering Committee June meeting	Q2 2022
	Arrange internal project meetings with funded CCPs and HECs – July 2022 – meetings arranged by scientific field	Q3 2022
	Compile and submit ARCHER renewal proposal	Q3 2022
	Arrange internal project meetings with funded CCPs and HECs – October 2022 – meetings arranged by scientific field	Q4 2022
	Prepare and submit interim CoSeC SLA report – November 2022	Q4 2022
	Arrange and attend the CCP Steering Panel December meeting	Q4 2022
	Attend the CoSeC SLA Steering Committee December meeting	Q4 2022
	Arrange internal project meetings with funded CCPs and HECs – January 2023 – meetings arranged by scientific field	Q1 2023
	Financial forecast and costing for 2023-24	Q1 2023
Impact	Re-design, maintain and update CoSeC web site	Ongoing

	Write and publish news articles and case studies on the CoSeC website	Ongoing
	Facilitate CCP/HEC website migration from Drupal 7	Ongoing
	Administrate CoSeC Impact Award	Q2 2022 – Q1 2023
	Design CoSeC branded (and environmentally sustainable) publicity and outreach material for workshop/conference handouts	Q2 2022 – Q4 2022
	Write and publish CoSeC Impact Award 2022 case studies	Q3 2022 – Q4 2022
	Launch the CoSeC Impact Award 2023	Q4 2022
Technical	Scope new working group areas and facilitate their start and goals	Ongoing
	Continue to drive existing thematic working groups (e.g. code coupling)	Ongoing
	Scope and create internal CoSeC skill-sharing exercises.	Ongoing
	Organise and run initial event as part of wider Computing Insight UK conference	Q4 2021
	Create new internal CoSeC event committee	Q1 2022
	Scope and design stand-alone CoSeC event	Q2 2022
	Scope new CoSeC open journal special edition as outlet for annual conference	Q2 2022
	Explore CoSeC curated journal special edition linked to annual meeting.	Q2 2022
	Scope and produce tangible outputs from working groups where appropriate (i.e. white-papers, group publications etc.)	Q3 2022
	Deliver first annual stand-alone CoSeC conference	Q4 2022
	Curate and deliver open journal special edition on computational sciences across CCP and HEC remit	Q1 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
	Lead PSDI Pilot WP2: Stakeholder Engagement	Q1 2022

Materials Science

CCP9	Milestone	Target Date
	Wannier90 developer meeting: presentation of new library	Q2 2022
	SPR-KKR Study of Ru based Heusler alloys	Q2 2022
	Questaal 7.16 release	Q2 2022
	CCP9 community meeting	~~Q2 2022~~ Q3 2022
	Compton profiles assessment phase	Q3 2022
	CRYSTAL parallelization extended to CPKS equations	Q3 2022
	MSSC2022	Q3 2022
	CRYSTAL22 release	Q3 2022
	Wannier90 “next version” including python interface	Q4 2022
	BSE – DMFT comparison study and paper	Q1 2023
	~~Casino – new Hire~~	~~Q1 2023~~

CCPNC	Milestone	Target Date
	Maintenance and further development of CCP-NC database	Ongoing
	Organise quarterly CCP-NC Online Meeting Series	Ongoing
	Maintenance and expansion of MagresView 2.0 based on community feedback	Q1 2023
	Complete review of programmatic tools for NMR crystallography in the light of community feedback.	Q3 2022
	CASTEP Workshop	Q3 2022
	Maintenance of the CASTEP-ASE interface: complete refactor of the input/output modules	Q3 2022
	Reimplementation of the SODORG code	Q1 2023
	Start industrial engagement placement programme	Q2 2022

UKCP	Milestone	Target Date
	Maintenance of CASTEP user licensing and source code distribution.	Ongoing
	Maintenance of CASTEP code repository and continuous integration system.	Ongoing
	Co-organization and teaching of CASTEP workshop(s).	Q3 2022
	Organisation of 2023 CASTEP "codefest" core developer workshop.	Q4 2022
	Release management of CASTEP v23 including documentation and liaison with major HPC services.	Q1 2023
	Extension of libXC interface in CASTEP for higher functional derivatives in TDDFT, Raman and NLO functionality.	Q1 2023
	Prototype implementation of van der Waals DFT (Dion) functional in CASTEP.	Q1 2023
	Port and release of Genetic Algorithm tool to coincide with academic CASTEP v22.	Q2 2022
	Coordination of new user documentation site alongside launch of ORCiD-authenticated CASTEP download web page.	Q3 2022
	Produce interface for CASTEP to YAMBO.	Q4 2022

MCC	Milestone	Target Date
Benchmarking	Complete comparison of non-bonded interactions in LAMMPS and DL_POLY, report to MCC	Q1 2022
	Comparison of bonded interactions in LAMMPS and DL_POLY, report to MCC	Q3 2022
	Specify codes and test cases for DFT comparisons in consultation with MCC (possibly CRYSTAL and CP2K)	Q2 2022
	Initial results for DGFT comparisons	Q4 2022
CRYSTAL	Installation (Q1 2022 tbc), testing and support for the new release of CRYSTAL for MCC members	Q4 2022
	Investigate the use of alternative distributed memory linear algebra software on ARCHER2	Q2 2022

ChemShell / DL-FIND	Set up and validation QM/MM of covalent materials with LSDalton	Q3 2022
	New release of Py-ChemShell	Q4 2022
	Interface to MolSSI basis set library for automated input of QM basis sets	Q1 2023
	Integration and validation of ML optimisation methods into DL-FIND release	Q1 2023
	Port, optimise and maintain ChemShell on ARCHER2 and Tier 2 systems (e.g. YOUNG)	Ongoing
DL_POLY	Investigate and optimise performance and scalability of short-range forces evaluations in DL_POLY_5.	Q3 2022
	Re-engineer the frozen-frozen coulombic interactions exclusion routine to be exact for large systems (and avoid discrepancies between virial and energy due to an implementation that approximates the interactions due to memory requirements).	Q4 2022
	New website set-up and launch	~~Q2 2022~~ Q3 2022
DL_FIELD	Improve automation of organic-inorganic non-bonded interactions - Interconversion of potential functional forms	Q4 2022
	Implement COMPASS force field (for general organic molecules in condensed phase) and general maintenance of existing libraries	Q3 2022
	Software release version 4.9 (including testing, manual updates)	Q4 2022
	Extend DL_FIELD capability to access to other third-party force field providers	Q1 2023

Biological Science

CCPBioSim	Milestone	Target Date
	Add modules to the online training and lead/support workshops.	Ongoing
	Maintain cloud infrastructure.	Ongoing
	CCP short project #2, part 2 (TRex/Pinda). Dec 2021-Feb 2022	Q1 2022
	CCP short project #3. Poseidon – a new tool for calculating entropy. Sept – Nov 2021, Mar – May 2022.	Q2 2022

	Review status of legacy codes (e.g. FESetup), former flagship projects and completed short projects and decide on future long-term maintenance levels for each.	Q3 2022
	CCP short project #4. To be determined by the management group after call for proposals. Starts June 2022	Q4 2022
	Implement full FFEA physics in CDO form within Code_Saturne.	Q1 2023
	Plan for the 5th Manchester Multiscale Conference.	Q1 2023
	CCP short project #5. To be determined by the management group. Starts Dec 2022	Q2 2023

HECBioSim	Milestone	Target Date
	Support the consortium users of HPC with ARCHER2, JADE, 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 T1 and T2 HPC	Ongoing
	Maintain HECBioSim webserver and website	Ongoing
	~~Maintain cloud based web and training infrastructure~~	~~Ongoing~~
	Update HEC website to Joomla 4 framework along with a refresh of look and feel	~~Q2 2022~~ Q3 2022
	Add Sulis and Wilkes3 to list of supported machines and start benchmark profiling	Q2 2022
	Link benchmark suite data output with resource calculator.	Q3 2022
	Complete release of Longbow 2022.0	Q4 2022
	Scope: Investigate adding OpenMM and BioSaturne benchmarks to benchmark suite.	~~Q1 2023~~ Q3 2022
	Scope: Investigate collaboration on assessing and improving access and performance for AI driven simulation	Q4 2022
	Scope: Investigate collaboration on assessing and improving access and performance for large scale enhanced sampling methods.	Q1 2023

Computational Engineering

UK-COMES	Milestone	Target Date
DL_MESO	Creation of HiLeMMS interface for DL_MESO_LBE code	Q1 2023
HiLeMMS	Explore the C++ template metaprogramming technique for automatically integrating contributions	Q1 2023
HiLeMMS	Initial integration of AMReX code for adaptive mesh refinement capability	Q1 2023

CCP-WSI+	Milestone	Target Date
	Integrate ParaFEM stand-alone structural solver into parMupSiF framework (creating new CCP-WSI+ framework).	~~Q2 2022~~ Q4 2022
	Website ported to new platform.	~~Q2 2022~~ Q4 2022
	Extend ESI OpenFOAM dynamic load balancing libary to work with the other moving mesh classes.	Q2 2022
	Port ParaSiF OpenFOAM-based FSI solver (interFSIFoam) to CCP-WSI+ ESI OpenFOAM code base.	Q2 2022
	Publicly release a generalised WSI software framework with effective FSI capability that can be extended for the CCP-WSI+ community and able to be delivered in a sustainable manner across platforms.	Q3 2022
	Software Catalogue prototype release.	Q3 2022
	Data Repository Development and maintenance.	Q3 2022
	Integrate capability of CCP-WSI+ waveFoam solver into ported interFSIFoam solver.	Q4 2022
	Directly integrate MUI coupling library into future ESI OpenFOAM releases (in collaboration with ESI).	Q1 2023
	Explore integration of MUI-enabled overset mesh capability from ARCHER2 eCSE project (finishes October 2022) into CCP-WSI+ software stack.	Q1 2023
	Software audit report.	Q1 2023

CCP NTH	Milestone	Target Date
	Add and validate conjugate heat transfer simulation into CHAPSim2	Q3 2022
	Add and validate embedded boundary method into CHAPSim2 for complex flow	Q1 2023

UKCTRF	Milestone	Target Date
	Implement the transverse and diffusion terms in NSCBC boundary condition for SENGA 2	Q2-Q3 2022
	Contribute to testing SENGA2 and HAMISH on ARCHER2 for 3D reacting flows and other validation studies	Q4 2022 - Q1 2023

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

CCP Turbulence	Milestone	Target Date
	CCP-turbulence to help in the organisation of the international event of ParCFD2022 and the CECAM school on CFD and HPC. Both will be held in Italy.	Q2 2022
Open SBLI	Implement the infrastructure for generating the implicit scheme codes	Q2 2022
Xcompact3d	Transfer of the GPU porting from the mini-app into the main branch of the code.	Q3 2022
OPS	Implement the linear algebra solver for the OPS code	Q1 2023
Xcompact3d	Porting of the xcompact3d mini-app to GPUs targeting hybrid heterogeneous applications.	Q1 2023

Tomographic Imaging

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives	Ongoing
	Organise exec 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 CCPSyneRBI	Ongoing
	Providing support for iterative reconstruction at facilities CLF/EPAC	Ongoing
	Further development of CIL with priorities set with the CCPi exec/steering panel	Ongoing
	Collaboration: Working with Brian Bay (USA) on improving and enhancing the digital volume correlation code	Ongoing
	Development of tools for GUI and interaction/visualisation of scientific data (CILViewer)	Ongoing
	~~Organise hackathon for development of novel reconstruction algorithms and benchmarking~~	~~Q4 2021~~
	Release of the digital volume correlation code and distributing it to CCPi community	Q1 2022
	Publication of a scientific article based on work enabled by CCPi Digital Volume Correlation	Q1 2022
	Release of simplified optimised reconstructor routines for cone beam and parallel beam CT in CIL, including FDK and iterative reconstruction with regularisation	Q2 2022
	~~CIL as Savu Plugin for parallel beam tomography~~	~~Q4 2022~~
	~~Code optimisation and restructuring of the CCPi Regularisation toolkit~~	~~Q1 2023~~
	Investigation of ML/AI methods for tomography	Q1 2023
	Investigate use of CIL with Electron Microscope data. COVID-19 study.	Q1 2023

CCPSyneRBI	Milestone	Target Date
	~~Example interfaces to Machine Learning framework(s).~~	~~Optional~~
	PET TOF support	Q3 2022
	PET List mode reconstruction for static data	Q3 2022
	~~Joint motion and reconstruction estimation (via connection with CIL).~~	~~Q4 2022~~
	More MR sequences	Q4 2022
	Creation of gated PET sinograms from listmode	Q1 2023
	Software performance improvements, including GPU support	Q1 2023
	~~MR reconstruction with PET prior (via connection with CIL).~~	~~Q1 2023~~
	~~Handling dynamic/gated data with parametric models.~~	~~Q1 2023~~
	Optional: Functions to compute gradients and values of MR objective functions.	Q1 2023
	Optional: PET-MR reconstruction using MATLAB or Python tools/toolboxes.	Q1 2023
	Example interfaces to Machine Learning framework(s).	Q1 2023
	First prototype of XNAT integration of docker-based pipelines	Q1 2023

Atomic and Molecular Physics / Plasma Physics

HEC Plasma	Milestone	Target Date
	Further follow-up and additional work with UK-AMOR depends on effort availability and UK-AMOR activity, but is highly desirable.	Ongoing

UK-AMOR	Milestone	Target Date
	Attend UK-AMOR management committee meetings as required and follow up accordingly. If funding allows, support workshop organization as appropriate (jointly with other CCPs/HECs, such as follow-up to the joint meeting on plasma applications of AMO physics).	Ongoing

	Follow-up existing plans and look out for new sources of funding to support UK-AMOR core support. In particular, support the HEC Renewal Call.	Ongoing
	As effort allows, carry out research in support of UK-AMOR science and codebase: this may involve follow-up RmatReact work related to the antimatter proposal and the 2021-2022 Graduate project, particularly if/once the antimatter proposal is successful. The highest immediate priority is to provide additional support for the AQuA-DIP project, which is entering is final year (for DL and QUB), and follow-up work on the RMT code eCSE project (which finishes at the end of May 2022).	Ongoing
	Keep track of any further UK-AMOR related outcomes of AGS's work	Ongoing
	Assuming successful renewal, decide on new objectives for Q1 2023 and 2023-2024	Q1 2023

Quantum Computing

CCP-QC	Milestone	Target Date
	Kickstart work on a new working group	Q1 2022
	Executive committee	Q2 2022
	WG2 workshop Q2 (London)	Q2 2022
	Executive committee	Q3 2022
	Crystallograpy working group	Q3 2022
	EPS Workshop	Q3 2022
	Executive committee	Q1 2023
	General training QC for computational scientists	Q1 2023

Appendix – Code Development

This appendix contains updates on code developments during 2021-22.

Materials Science

CCP9	Code Development	Comments
Wannier90	1. Type definition and classification 2. Error handling 3. "librification"	1. Complete 2. Complete 3. Ongoing
QUESTAAL	Spin-dependent susceptibilities in BSE	Ongoing

CCPNC	Code Development	Comments
MagresView 2.0	Structured the basic React-based framework for the site, developed customised interface and UI controls	Complete
Soprano	1. Released version 0.8.11 2. Development of a class to compute dipolar fields in presence of random magnetic dipoles	1. Complete 2. Ongoing
CASTEP	1. Redeveloped transition state capability 2. Added a socket driver functionality that allows CASTEP to be connected to the i-Pi framework for complex meta-calculations of transition states as well as classical and quantum dynamics.	Complete with funding from the ARCHER2 eCSE project and supported by the CCP-NC.

MCC	Code Development	Comments
ChemShell	1. Interface to Molpro 2. Port to ARCHER2 using GNU compilers	1. Complete 2. Complete
DL_POLY	Code review and port to ARCHER2	Complete
DL_FIELD	1. Improvement on the use of xyz file format for organic and inorganic systems. (Ease of use and improvement to integrate with ChemShell). 2. Auto-mixing and setup vdw interactions using Slater-Kirkwood formalism. (Workflows for setting up mixed complex systems) 3. Solvation using solvents from different force field libraries for both single potential and multiple potential settings (for PDB and xyz structures).	1. Completed 2. Completed 3. Completed
CRYSTAL	CRYSTAL is currently in a code freeze undergoing testing for a major release early in 2022	

Biological Science

CCPBioSim	Code Development	Comments
Enlighten	Added link to ChemShell for QM/MM capability	Complete
BioSaturne	Merged the steady and unsteady implicit parts of the equations. This required adding a new subroutine to account for the temporal terms for vectors.	Ongoing
Posiedon	Parser in CodeEntropy has been replaced by functionality from the widely popular MDAnalysis package. An alpha version of CodeEntropy has been produced and preparations of merger with Poseidon is underway.	Ongoing

HECBioSim	Code Development	Comment
Longbow2.0	1. Restructure code base into more modern library approach 2. Added in functionality to allow password-less use of very secure machines 3. New lightweight GUI mode 4. Native support for Chemshell 5. Native support for DL_Poly 6. Support for ARCHER2, JADE2 and Bede 7. Better support for newer architectures 8. Slurm scheduler plugin significantly expanded	The features listed here are currently a work in progress but describe some of the functionality that is already being added to the new release in the current reporting cycle.
Resource Calculator Applet	1. Data model constructed to forecast HPC resource requirements for multiple machines. 2. Energy consumption forecasting model introduced to give energy use estimates. 3. Containerised data model to run on k8s infrastructure. 4. New front end for user input to display more complex data due to difference in machine architectures.	Complete

Computational Engineering

UK-COMES	Code Development	Comment
DL_MESO	1. Implementation of (three-dimensional) fluid-filled vesicle algorithm in LBE code 2. Addition of multiple-phase interaction types to DPD code 3. New GUI for simulation setup and post-simulation analyses	1. Complete (Q1 2022) 2. Complete

		3. Ongoing, should complete by Q2 2022
MPLB	Development of free-energy model (as part of CCP5 summer project)	Complete

CCP-WSI+	Code Development	Comments
Software Catalogue	Development to CCP-WSI+ requirements: 1. Schema 2. Search interface 3. Front end software page 4. Front end projects page 5. Admin page 6. Deployment to working group for testing	 1. Complete 2. Complete 3. Complete 4. Complete 5. Complete 6. In-progress
ParaSiF	1. Release as open source on GitHub 2. Port and compiled on ARCHER2 3. Port and compiled on SCARF 4. Integrate ParaFEM from OpenFPCI 5. Develop *interFSIFoam* solver from ParaSiF to include *waveFoam* functionality	1. Complete 2. Complete 3. Complete 4. Underway 5. Underway
ParaFEM Solver	1. Define requirements for stand-alone solver 2. Create new solver based on latest ParaFEM 3. Package ParaFEM using Spack 4. Integrate new solver into ParaSiF	1. Complete 2. Underway 3. Underway 4. Underway
Multiscale Universal Interface code coupling library	1. Maintain and support library 2. Develop parallel performance of library for use on highly-parallel architectures like ARCHER2 3. Integrate the library fundamentally into ESI OpenFOAM (working with ESI to formalise into future releases)	1. Ongoing 2. Ongoing 3. Ongoing
ccp-wsi-new Repository	1. Restructure the code to use the latest ESI OpenFOAM releases 2. Improve code mainability by remove redundant code	1. Underway 2. Complete
decomposePar (ParMETIS)	1. Create as stand-alone library/application (rather than patch for specific OpenFOAM versions) 2. Integrate into various CCP-WSI+ repositories	1. Complete 2. Underway
ESI OpenFOAM load-balancing capability	1. Create first instance of new ESI OpenFOAM Class 2. Refine and further develop for general use	1. Complete 2. Underway

CCP NTH	Code Development	Comment
The library 2DECOMP&FFT	Test of built-in FFT sub-library and different third party FFT libraries, for instance, FFTW, to validate its functions before implementation in CHAPSim2.0	Complete
CHAPSim2.0	1. Application of the library '2DECOMP&FFT' to CHAPSim2.0 in serial mode. 2. Application of the library '2DECOMP&FFT' to CHAPSim2.0 in parallel mode 3. Function of CHAPSim2.0 in decomposing computational domain into pencil sub-domain and transposing pencil sub-domain into different directions 4. Function of CHPASim2.0 to solve a Poisson equation with three-dimensional Fourier Transformation 5. A Taylor-Green Vortex case tested to validate the feasibility 6. Test of Burger's equation using the developed CHAPSim2. in parallel mode 7. Test of Poisson equation using various boundary conditions in parallel mode	1. Complete 2. Complete 3. Complete 4. Complete 5. Complete 6. Complete 7. Ongoing

UKCTRF	Code Development	Comment
rhsvel.f rhscal.f	Extensive lines are added in the exsiting subroutines to collect information for the boundary conditions.	
bound_outflow_faces.f bound_outflow_xedge.f bound_outflow_yedge.f bound_outflow_zedge.f bound_outflow_corners.f	New subroutines are created to replace the original boundary subroutine bound.f	

UKTC	Code Development	Comment
Xcompact3d	Scope out integration of particle tracking into the code	Limited scoping exercise that was stopped due to FTE reduction.

CCP Turbulence	Code Development	Comment
OPS	A new documentation framework is created https://ops-dsl.readthedocs.io.	Existing manual is being transformed.
OPS	New applications for the OPS library.	Demonstrating the usage of tridiagonal linear solver and implementing the compact scheme in C/C++.
Xcompact3d	Merge of the https://github.com/rfj82982/Incompact3d into the Master branch of the code	Merge to be finalised to verify that code performance has not been degraded.
X3div	Full multi-GPU porting with CUDA aware, MPI or NCCL and for communication and cuFFT for the Poisson solver https://github.com/xcompact3d/x3div/tree/cuFFT_fortran	Completed on development branch. To be merged in master branch.

Tomographic Imaging

CCPi	Code Development	Comments
CIL	1. Plugin for TIGRE engine - allows comparison of different engines, such as ASTRA 2. Processors to determine centre of rotation - this is a fundamental step in the analysis of the tomographic data 3. Development of readers for ZEISS, NIKON lab machines - data readers are fundamental and we are adding new functionality constantly 4. Development of optimised analytical reconstruction method with TIGRE projectors - enables faster, more memory efficient and versatile FBP/FDK algorithm (the most common algorithm for reconstruction)	
DVC	Addition of code to calculate strain	
CILViewer	Enable visualisation of arbitrarily large dataset by downsampling.	

CCPSyneRBI	Code Development	Comments
SIRF	1. Add PET scatter estimation. 2. Enable reading GE Signa PET/MR data 3. Implement the extraction of the linear part of PET acquisition model and computation of its norm (required by CIL algorithms). 4. Optimize the handling of STIR memory-stored PET acquisition data by taking advantage of direct access to it provided by STIR. 5. Simplify the handling of MR coils images and sensitivities in C++ by deriving respective classes from the abstract base class MRImageData. 6. Provide support for the MR radial phase encoding if Gadgetron toolboxes are available. 7. Drop Python 2 support. 8. Replace Travis CI with GitHub Actions CI 9. Make unsuccessful data validity checks return NotImplemented rather than throw error to allow possible future implementations of operations on data.	Complete

Atomic and Molecular Physics / Plasma Physics

HEC Plasma	Code Development	Comments
Bout++	Bugfix and new release: https://github.com/boutproject/BOUT-dev/releases/	

UK-AMOR	Code Development	Comments
RMAT_REACT	Over the course of UK-AMOR, develop a bound state code (and possibly a resonance code) for low temperature atom-atom (molecule-molecule) reactive collisions, adapting existing code from the electron-molecule UKRMol(+) package and the TIMEDELn time-delay package. *Initial interfacing work for data transfer, as adapted for collision code PFARM, for the preferred bound state code has been examined and adapted for rearrangement channels as part of the new Graduate project (supported by MP) in September-March (and in preparation for the antimatter work). RmatReact work was also included in the Software for Research Communities proposal.*	Ongoing The Graduate project has investigated the mixed coordinate systems needed for the R-matrix (bound and quasi-bound) inner region and links to the separate coordinate systems for each arrangement outer region on the boundary hypersurface. A code for numerical integrals transforming between coordinates (with correct inner intergral limits) has been written.
PFARM	AGS has started porting PFARM to the current range of PRACE Tier-0 architectures (CPUs/GPUs) (to progress in earnest by beginning of November). Energy usage monitoring will be a much more significant factor in these benchmark results. The benchmark framework (documentation, run setup scripts and job submission setup scripts) for CPU and GPU runs has recently been developed for the latest release of the UEABS and this has been independently tested by two research groups in Barcelona and Ankara. https://repository.prace-ri.eu/git/UEABS/ueabs	Work done as part of a PRACE project obtained as a result of UK-AMOR/CCPQ core support.

Appendix – Training and Outreach

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

Materials Science

CCP9

CoSec supported training/outreach:

- CRYSTAL virtual workshop "MSSC2021-Virtual Ab-initio Modelling in Solid State Chemistry", 20-24 September, London. Barry Searle was tutoring at the course.
- CCP5 Summer school, 11-22 July, 2021, online. Barry Searle gave 2 lectures (36 students) and participated in the tutorial sessions of advanced course on first-principles simulation, 20-22 July.
- Computer Physics Communications seminar on July 27, online, presented by Jerome Jackson. "Questaal: A package of electronic structure methods based on the linear muffin-tin orbital technique"
- Posters presented at Ecole de Physique Les Houches : Jerome Jackson , "QUESTAAL : A package electronic structure codes based on the LMTO technique", and Leon Petit "Complex magnetism of Gd-intermetallics"
- "A practical approach to applying PZ-SIC to solids", invited online presentation given by Leon Petit at the International Conference on Recent Advances in High Pressure Science and Technology, IGCAR, India, 8 February 2022
- "SPR-KKR hands-on course on magnetism and spectroscopy", 22-25 November 2021, Daresbury Laboratory. Jerome Jackson and Leon Petit organizing and tutoring
- Workshop on "Data enabled atomistic modelling", 18-19 November 2021, Coseners House. Leon Petit co-organizing with Alin Elena (CCP5+)

CCP9 provided funding for:

- "Integrating Quantum Computers in Condensed Matter Physics Simulations", National Physical Laboratory, 23-24 September 2021

No further funding was requested by members of the CCP9 community for organizing workshops during this periods, as all activities have been either postponed, or were organized as virtual workshops.

During the 20/21 period four Psi-k highlights were edited and published https://psi-k.net/highlights/:

- Non-linear response of solids and nanostructures: a real-time prospective, by C. Attaccalite et al.
- DFTB+, a software package for efficient approximate density functional theory based atomistic simulations, by B. Hourahine et al.
- The CECAM Electronic Structure Library and the modular software development paradigm, by MJT. Oliveira et al
- Atomic Simulation Recipes - a Python framework and library for automated workflows, by M. Gjerding et al.

CCPNC

The CASTEP workshop, which would normally have been run in person in August, was again cancelled due to the COVID-19 pandemic.

Given the limited opportunities for travel in 2020-21, EPSRC approved the use of unspent travel funds for a summer studentship (Aug and Sep 2021). This was extremely effective in helping to populate and stress test the magres database.

Kane Shenton has been principally involved in outreach and training from the start of his full-time position in October. This has involved understanding and discussing the needs of users, setting up an online community platform, and co-organising a new online discussion meeting series, the first of which is to be held on the 6th of April 2022. A communication strategy document was also produced as part of this outreach refresh.

A need for improved documentation and tutorials was identified through this user consultation and some work towards creating these has been carried out. Documentation on dispersions corrections to density functional theory has been contributed to a new CASTEP documentation website.

A new case-study page has been added to the CCP-NC website, with contributions from members of the community being coordinated by Kane.

The expression of interest call for our Industrial Engagement PDRA position has generated bids from three major companies, which augurs well for the industrial outreach programme.

MCC

- 24 May 2021 – MMM DDWG community discussion of scientific case studies for exascale computing platforms
- 8 June 2021 – Ian Bush, Alin Elena and Tom Keal participated in the ExCALIBUR High Priority Use Case workshop
- 23 September 2021 – Ilian Todorov, Tom Keal, Kakali Sen and You Lu provided an introduction to the DL_Software suite and training on QM/MM methods using ChemShell at the PRACE Autumn School 2021, with a mix of presentations and live demos.
- 20-24 September 2021 – Ian Bush, Barry Searle took part in MCCS2021 introducing the use of CRYSTAL to new users
- 4 February 2022 – Ilian Todorov, Alin Elena, Michael Seaton and Chin Yong introduced DL_POLY, DL_MESO and DL_FIELD to new users at the PRACE Winter School 2022 in Sofia
- 14-15 March 2022 – PAX-HPC all hands project meeting held at Daresbury, bringing together the MMM and MPPH communities to discuss the Excalibur phase1b project work packages.

Biological Science

CCPBioSim

- Advanced Course “Simulating Biomolecules” at the CCP5 Summer School, online, 20-22 July 2021.
- CCPBioSim Training Week, online, 28 September – 4 October 2021.

HECBioSim

None delivered in the reporting year due to the arrival of many new architectures.

Computational Engineering

UK-COMES

Michael Seaton contributed to the CCP5 Summer School in July 2021, previously postponed from 2020 and held online (18 participants over three days), and to the online Introductory PRACE Course “HPC Fundamentals for End-Users” in February 2022 (up to 40 participants for one day). This included seminar talks and practical exercises using DL_MESO for both DPD and LBE. Michael has been contributing material on DL_MESO and mesoscale modelling (DPD and LBE) to the DL_Software Digital

Guide, an online training guide for new and existing users of DL_Software packages (https://dl-sdg.github.io/). He is also collaborating with Tim Reis (Greenwich) to implement a new moment-based boundary condition into the LBE code.

Jianping Meng provided training to Mr Michael Rennick on the HiLeMMS and the MPLB backend for the CCP5 summer project.

CCP-WSI+

7-8th April 2021: Code Developer's Workshop 2: Significant CoSeC interaction to help organise and define the virtual event, including speaker invitation. Talk given by CoSeC staff member Stephen Longshaw on "Generalised Scientific Code Coupling Using the Multiscale Universal Interface Library".

13-14th October 2021: Code Coupling Workshop: CoSeC organised virtual workshop on generalised code coupling with a focus on practical use of the Multiscale Universal Interface code coupling library.

CCP-NTH

Special topic seminars are carried out via Zoom as planned. In the last quarter (29th June), we organized the "Topic: Multi-phase flow and boiling" special topic seminar with speakers from Paul Scherrer Institute, ETH Zurich and University of Leeds.

A training course on Nek5000 has been co-organized by CCP-NTH and Argonne National Laboratory (ANL), which ran on 15th and 16th December 2021. Nek5000 is an open-source spectral element-based CFD code to simulate unsteady incompressible fluid flow with thermal and passive scalar transport. This training course comprised a mixture of lectures and tutorials.

The CCP/SIG NTH 2021 Annual Technical Meeting was held in December 2021. The Technical Meeting comprised an update on the CCP-NTH work packages 1 and 2, followed by a keynote talk, and short and extended presentations from the community about recent R&D/research activities.

CCP-NTH was involved in the CoSeC Annual Conference 2021. Wei gave a talk about "Nuclear thermal hydraulics for low-carbon applications – understanding energy and mass transport in advanced nuclear reactor systems".

Users of CHAPSim2 and GPU experts from the Hartree Center have formed a team for extending CHAPSim2 to GPU in the 3-day training even of the CoSeC GPU Hackathon. (10-12 Jan 2022).

CCP-NTH and CCP-Turbulence keeps close contact, especially in the development and application of the 2DECOMP&FFT libraries. CCP-NTH community was also involved and contributed to the Physical Sciences Data Infrastructure (PSDI).

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-NTH has gone live... https://ccpnth.ac.uk.

UKCTRF

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

UKTC

Preparation for training course in April for UKTC core code: HPC for CFD using Code_Saturne, Charles Moulinec (STFC), Juan Uribe (EDF), 27 - 28 April 2022.

CCP Turbulence

A periodic hackathon event to bring the Xcompact3d development community together is on-going every 3 months. The event is organised by the CCPTurbulence chair (Dr. S. Laizet) and S. Rolfo and C. Moulinec are regular attendee and contributors. This semester events were: 21 June, 28 September.

A major hackathon has been organised by the CCP-Turbulence in collaboration with NVIDIA, CCP-NTH and CCP5++ to port modern Fortran codes to multi-GPU. (10-13/01/2022)

CCP-Turbulence has also participated to the UKRI GPU hackathon on 27/02/2022-09/03/2022. The results of the two hackathons is the full porting to multiple GPU(s) of the X3div mini-app.

Tomographic Imaging

CCPi

The team has been working at organising a joint Training School for the Synergistic Image Reconstruction Framework (SIRF) and Core Imaging Library (CIL) | CCPi Tomographic Imaging, with CCP-SyneRBI, attached to the Fully3D international conference. The training has been attended by about 50 trainees over 3 weeks.

The team efforts have been devoted to all aspects of the training, from the creation and organisation of the training material, to the set-up of the training platform on the SCD cloud, from the initial organisation to the user support over the 3 weeks of the training.

Two smaller scale online training events have been done, one at the ToScA conference, and one online, with 13 and 26 trainees respectively.

A discord server was launched to better reach and interact with CIL users. These include both those using CIL as an optimisation problem framework, and CT users looking for open-source maintained solutions. Approximately 50 users have joined, and new users have actively engaged with the team.

CCPSyneRBI

Our main outreach activities during the reported period continued to be our regular Software Framework meetings, where we discussed our development progress with our developers and potential users from Biomedical Research community (KCL, Leeds, Manchester, PTB Berlin, and other Universities' researchers) and representatives of major imaging scanner manufacturers, including Siemens and GE.

Our main training activity was the online 3-weeks training course provided from 28 June to 16 July 2021 with 3 live Zoom sessions per week. This was organised together with the CCPi team as well as many people within the SyneRBI network. This course covered SIRF together with the image reconstruction, optimisation and regularisation software library CIL (Core Imaging Library) of the CCPi

team. The course was taken by 50 people, 15 of which were very active and 20 left positive feedback. Several new developments were put in place including ability to deploy on the STFC Cloud using JupyterHub. This course and its material will provide the foundation for future training courses but also for self-training. The subjects covered were as follows

- Week 1: Basic components for PET, MR, CT
- Week 2: Iterative reconstruction and regularisation
- Week 3:
    - Synergistic reconstruction
    - Deep learning for post-processing of PET images using MR side information

Atomic and Molecular Physics / Plasma Physics

HEC Plasma

A major training event was the 'Atomic and Molecular Data Needs for Plasma Applications' workshop, with 23 talks informing and educating the AMO and plasma/fusion communities on each other's work (this training was reported in the UK-AMOR report).

UK-AMOR

Training activities provided by SLA/CoSeC for UK-AMOR and CCPQ members are generally in the form of specialized informal group meetings and one-to-one interactions (local and virtual). In this reporting period there have been 'scientific code' discussions on various topics, in particular on the adaptation of RmatReact for antimatter and rearrangement collisions. STFC Graduate Elliott Kasoar has been trained in collision theory and HPC scientific programming as part of his 6-month rotation project. A major training event was the 'Atomic and Molecular Data Needs for Plasma Applications' workshop, with 23 talks informing and educating the AMO and plasma/fusion communities on each other's work. [Discussions on multiphoton topics, electron-atom interactions and the RMT code took place as part of other projects (the eCSE and the AquA-Dip grant) obtained as part of UK-AMOR/CCPQ work, and on antimatter and RmatReact as part of the Graduate project.].

Quantum Computing

CCP-QC

Alin Elena was invited to the ground breaking ceremony at the National Quantum Computing Centre site.

Underpinning Technologies

Software Outlook

As part of the code coupling work, Philippa Rubin gave a SCD Seminar on "Code Coupling Libraries for High Performance Multi-Physics Simulation". This was advertised to all of the CCPs and HECs, and there was an audience of over 50 people. Philippa's accompanying report also contains training material on the use of different code coupling libraries.