EPSRC Service Level Agreement with STFC for Computational Science Support

FY 2017/18 Annual Report and
Update on FY 2017/18 Work Plans

June 2018

Table of Contents

Background

The Scientific Computing Department (SCD) of the Science and Technology Facilities Council (STFC) provides computational science support for a number of scientific communities funded by EPSRC, and organised in Collaborative Computational Projects (CCPs) and High End Computing (HEC) Consortia. This programme of work is carried out by staff at the Daresbury and Rutherford Appleton Laboratories under a Service Level Agreement (**SLA**) with EPSRC, and its main objectives are:

- Develop and maintain codes and methods to keep them internationally relevant for current and evolving scientific challenges and hardware capabilities
- Widen participation in the exploitation of methods and codes through training and scientific collaboration
- Support collaboration and coordination of the various communities to broaden and strengthen the UK-based research activities aligned with EPSRC's goals
- Provide career paths and professional development opportunities for computational scientists and engineers focused on method and software development
- Widen engagement with the broader UK and international communities engaged in developing methods and software for computational science and engineering

The nature of the support provided is tailored to the needs of the communities and can include:

- **Development of theory, algorithms, and software**: This is a key element of support for many current projects, resulting in long-term, continued expansion and updating of the software programs. It may include the consolidation of existing codes into a more sustainable community software package
- **User support and training**: This includes individual support and training as well as help to organise and conduct events such as workshops, summer schools and study weekends. Support for Centres of Doctoral Training is also offered
- **Outreach and promotion of computational science and engineering activities**: facilitate the exchange of expertise, and tools, reaching out to new communities, including experimentalists and industry, nationally and world-wide
- **Collaboration on scientific projects**: working together with scientists in the communities to advance scientific research and help nurture projects and develop new opportunities
- **Porting, optimisation, and benchmarking** on local and national computing platforms including High Performance Computing (HPC) and new architectures: evaluation of new hardware and software technologies
- **Maintenance, distribution**, license management, dissemination and demonstration of software
- **Management of scientific data**: This includes activities such as, for example, the development of visualisation and workflow management tools, database and archiving, and verification and validation activities
- **Co-ordinate and nurture existing and new communities**, from practical tasks such as organising community meetings, to representing the communities in strategic activities in the UK Research Councils and abroad.

CoSeC, the Computational Science Centre for Research Communities, brings together these activities with those in support of CCP4 (partly funded by a BBSRC grant), CCP-EM (funded by an MRC grant), and CCP-WSI (funded by an EPSRC grant): https://www.scd.stfc.ac.uk/Pages/CoSeC.aspx

The communities currently supported are summarised in the table below:

Project	Title	Project Chair	CoSeC Project manager
CCP5	The Computer Simulation of Condensed Phases.	Prof Neil Allan	Dr Alin Elena
CCP9	Computational Electronic Structure of Condensed Matter	Prof Stewart Clarke	Dr Leon Petit
CCP-Mag	CCP on Computational Magnetism	Prof Julie Staunton	Dr Martin Lueders

CCP-NC	NMR Crystallography	Dr Jonathan Yates	Dr Simone Sturniolo
CCPQ	Quantum dynamics in Atomic Molecular and Optical Physics	Prof Graham Worth	Dr Martin Plummer
CCP-Plasma	The Plasma-CCP Network	Prof Tony Arber	Dr Joseph Parker
CCPi	Tomographic Imaging	Prof Phillip Withers	Dr Edoardo Pasca
CCP-PET/MR	Computational Collaborative Project in Synergistic PET-MR Reconstruction	Prof Kris Thielemans	Dr Evgueni Ovtchinnikov
CCP-BioSim	Biomolecular simulation at the life sciences interface	Prof Adrian Mulholland	Dr Tom Keal
Materials Chemistry	UK Materials Chemistry Consortium	Prof Richard Catlow	Dr Tom Keal
HEC-BioSim	High-End Computing Consortium in biomolecular simulation	Prof Adrian Mulholland	Dr James Gebbie
UKCP	United Kingdom Car-Parrinello Consortium	Prof Matt Probert	Dr Dominik Jochym
HEC-Plasma	Plasma High-end Computing Consortium	Prof Tony Arber	Dr Joseph Parker
UK-COMES	UK Consortium on Mesoscale Engineering Sciences	Prof Kai Luo	Dr Michael Seaton
UK-AMOR	UK Atomic, Molecular and Optical physics R-matrix Consortium	Prof Jonathan Tennyson	Dr Martin Plummer
UKTC	UK Turbulence Consortium	Dr Sylvain Laizet	Dr David Emerson
UKCTRF	UK Consortium on Turbulent Reacting Flows	Prof Nilanjan Chakraborty	Dr David Emerson

A brief description of each community can be found in the community-specific sections below. More information is available at http://www.ccp.ac.uk/ for the CCPs and at https://www.epsrc.ac.uk/research/facilities/hpc/access/highendcomputingconsortia/ for the HEC consortia. The current level of support awarded to the communities is as follows:

Community	**Core support per project (FTEs per annum)**
CCP5	3.4
CCP9	2.6
CCP-Mag	0.8
CCP-NC	1.4
CCPQ	2.0
CCP-Plasma	0.8
CCPi	1.3
CCP-PET/MR	1.25
CCP-BioSim	1.25
Materials Chemistry	2.5 (2 from 31 Oct 2018)
HEC-BioSim	1.0 (0.8 from 31 Oct 2018)
UKCP	1.0

HEC Plasma	0.2
UK COMES	1.0 (0.6 from 31 May 2018)
UK-AMOR	0.2 (from 1 April 2018)
UKTC	0.3 (from 30 June 2018)
UKCTRF	0.13 (from 07 Jan 2019)

STFC News

Tom Griffin (currently Head of Computing for ISIS) will start his new job as Director of SCD on 2nd July 2018. He replaces David Corney who has partially retired. We thank David for a fantastic job at the helm of the Department for the last 4 years.

Following Barbara Montanari's promotion to Head of the Computational Science and Engineering Division last year, a new leader for the Computational Physics Group has been appointed and will start on 1st August: Dr Gilberto Teobaldi (currently at Liverpool university). This group provides CoSeC support for: CCPQ, UK-AMOR, CCP-NC, CCP9, MCC, UKCP, CCP-mag, CCP-Plasma and HEC Plasma.

On 1st April, STFC became part of UKRI. Prof Mark Thomson has been appointed as the STFC Executive Chair.

The STFC e-infrastructure strategy has now been published: https://www.scd.stfc.ac.uk/Pages/STFC-e-infrastructure-strategy-published.aspx

SCD received capital funding from BEIS for the IriS initiative, which brings STFC computing interests together mainly across particle physics, nuclear physics, astronomy, and the national experimental facilities. The bulk of the investment will be to increase compute and storage capacity across the large number of projects and partners involved, and break down barriers for sharing access.

The Data & Analytics Facility for National Infrastructure (DAFNI) project is in its second year. This is an investment from the UK Collaboration for Research on Infrastructure and Cities (UKCRIC). DAFNI aims to improve the quality and reliability of national infrastructure services, economic productivity, and its impacts upon the environment. SCD will be delivering the compute, data, and modelling platform for research on infrastructure systems.

NOTE: in the following reports the red text in the plans tables indicates an update on progress against individual tasks.Text highlighted in yellow indicates a change from the interim report submitted in December 2017.

CoSeC Project Office

The objectives of the Project Office are:

- 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
- 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.

Project Office – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

The project office will continue to support the CoSeC funded CCPs and HEC Consortia through a series of quarterly project meetings allowing a flow of information in both directions that will identify areas where support is required. Monitoring of effort and financial information will be undertaken by the project office support manager, who will additionally monitor CoSeC usage on ARCHER and report back to the CoSeC manager at regular intervals. A renewal for the CoSeC allocation on ARCHER will be submitted. We will engage in the preparations for the 2018 International mid-term review by preparing case studies in collaboration with our communities in order to highlight the impact that CoSeC enables though the CCPs and HEC Consortia that it supports.

Support for Drupal based CCP websites will continue and, with support from the CoSeC impact manager, the project office will explore options to increase the impact of the work completed by CoSeC funded projects. Plans are being made for a significant CoSeC presence at the Annual Research Software Engineering Conference (Manchester, September 2017), including a stand. The relaunch of the EPSRC SLA as CoSeC is also being planned for the autumn. The project office will also prepare and submit two reports to the SLA Steering Committee and EPSRC – an annual report covering the full twelve months of the 2016/17 financial year will be submitted in June and an interim report covering the first six months of the 2017/18 financial year will be submitted in December.

Project Office	**Milestone**	**Target Date**
	Attend CCP and HEC committee meetings as required Damian attended the last CCPQ committee meeting and presented on what the project office can do for that community. As a result CoSeC is now assisting with the practical arrangements for a CCPQ workshop to be held in 2018.	Ongoing
	Support CCP/HEC conferences and workshops as required Support has been provided to CCP5, CCPQ and CCPBioSim this year and discussions are ongoing with CCPi and UKCP about support for their upcoming events...	Ongoing
	Planning for the SLA International Review 2018 A number of activities were undertaken which are summarised in the report..	Ongoing
	Provision of technical IT support for SLA staff Support provided on demand.	Ongoing
	Planning for TSM Backup software update There is lots of documentation to go through. The backup is very complex. Viliam is preparing another machine to test the update before completing the process on the real machine.	Ongoing

	Management of user access to data infrastructure Problems can occur because machines for new starters are not provided on the correct sub-net. Viliam has mentioned this to IT Support.	Ongoing
	Maintenance and monitoring of data infrastructure There was a recent failure on the main board of the back-up server which was resolved quickly. This was a sign that the equipment is ageing but everything is under support agreement.	Ongoing
	Management of SCD subnet in cooperation with CICT In progress. Viliam has requested that group leaders inform him when they have new starters or people leaving so that he can manage this more efficiently.	Ongoing
	Provision of operation support (shifts) to Archer service In progress. Viliam covers shifts on ARCHER.	Ongoing
	Arrange internal project meetings with funded CCPs and HECs Complete Meetings held in April 2017	Q2 2017
	Prepare and submit annual SLA report Complete. Submitted on time in June 2017	Q2 2017
	Arrange and attend the CCP Steering Panel June meeting Complete. Meeting held on 26 June	Q2 2017
	Attend the SLA Steering Committee July meeting Complete. Meeting held on 17 July	Q2 2017
	Compile departmental data infrastructure usage data Complete. Viliam will send final version to Barbara.	Q2 2017
	Negotiate maintenance contract for data infrastructure hardware and software Complete. The contract is now agreed and in place.	Q2 2017
	Arrange internal project meetings with funded CCPs and HECs Complete. Meeting held in August 2017	Q3 2017
	Compile and submit ARCHER requirements Complete. Renewal proposal was submitted to EPSRC	Q3 2017
	Create new CoSeC web site Complete. The site is now live and will be updated and improved on an ongoing basis.	Q3 2017
	Update TSM backup software for data infrastructure (prerequisite) Ongoing. Reduced database to prepare for update	Q3 2017
	Deliver presence at the Research Software Engineering Conference (Manchester) Complete. Barbara presented at the conference 7-8 September	Q3 2017
	Prepare and submit mid-term SLA report Complete. Submitted December 2017.	Q4 2017
	Create new CCP web site using Drupal In progress. A template for the site is now in place and content from www.ccp.ac.uk is being copied across.	Q4 2017
	Prepare and submit tender for external impact report Complete. Tender submitted in October	Q4 2017
	Commission external impact report Complete. Report commissioned in November. Technopolis are the chosen supplier.	Q4 2017
	Prepare and deliver talk on CoSeC for the STFC Computing Advisory Panel	Q4 2017

	Complete	
	Prepare and deliver talk on CoSeC for the CIUK Conference Complete	Q4 2017
	Arrange and attend the CCP Steering Panel December meeting December 5th – JISC Complete	Q4 2017
	Attend the SLA Steering Committee December meeting Date TBC Complete. The meeting was delayed until January 2018 as a suitable date could not be found in December	Q4 2017
	Update TSM backup software for data infrastructure (final version) Complete	Q4 2017
	Procure new server for data infrastructure Ongoing	Q4 2017
	Integrate new server for data infrastructure Ongoing	Q1 2018
	Liaise with consultant to provide data and information for the external impact report Ongoing. Kick-off meeting held in December with regular meetings since. The activity began in March 2018.	Q4 2017 and Q1 2018
	Arrange internal project meetings with funded CCPs and HECs Complete. We took a change of approach to these meetings as we had a large amount of important information that we wanted to pass on. Instead of the usual individual project meetings we held one meeting for Daresbury project leaders and one for Rutherford project leaders to avoid having to repeat everything multiple times	Q1 2018
	Prepare 4 impact case studies Complete. This task was extended to invluce one project from each supported CCP and HEC.	Q1 2018
	Organise an internal CoSeC staff meeting Complete. The meeting will take place at Daresbury Laboratory on 30 April – 1 May 2018	Q1 2018

Staffing	**Effort (FTE)**
Mark Forster	~~0.05~~ 0.00 FTE
Damian Jones	0.70 FTE
Viliam Kalavsky	0.50 FTE
Marion O'Sullivan	0.25 FTE
Barbara Montanari	0.50 FTE
RIG Group	0.25 FTE
Total	**~~2.25~~ 2.20 FTE**

Project Office – Summary Report (1 April 2017 – 31 March 2018)

The project office have carried out major impact and outreach activities during the reporting period. The most important of these was the creation and launch of CoSeC which included: presence and a talk at the RSE Conference (Manchester, Sept 2017); a new logo, website, and press release; twitter activity (@CoSeC_community); and an interview for an article on Research Fortnight. Furthermore, a talk was delivered at the CIUK Conference (Manchester, Dec 2017); as part of the RSE International Leaders Conference, international RSE leaders visited the Rutherford Appleton Lab (29-31 Jan, 1 Feb 2018); CoSeC presence and presentations were coordinated for two SSI events: The "Collaborations Workshop" (Cardiff, 26-28 March 2018) and the "Workshop: Impact of international collaborations in research software" (Manchester, 24 April 2018).

Much activity happened around two reviews: the SLA International Mid Term Review commissioned by EPSRC and the review by the consultancy company Technopolis, commissioned by the CoSeC Director. Regarding the latter, an extensive survey has been circulated to the SLA communities and interviews to several SLA stakeholders are taking place. A partial report on four of the communities will be delivered by Technopolis in June. We expect the final report to be delivered in December.

During the current reporting period the project office has provided workshop support to CCP5, CCPQ and CCPBioSIm in the form of online registration forms, web pages and the collection of registration fees. Damian Jones has also started to attend some CCP committee meetings to present on what the project office can do for those communities. The work with CCPQ was as a direct result of one of these visits and will continue in to 2018 with support for a second CCPQ event,

Project Office – 2018/19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

The project office will continue to support the CoSeC funded CCPs and HEC Consortia through a series of quarterly project meetings allowing a flow of information in both directions that will identify areas where support is required. Monitoring of effort and financial information will be undertaken by the project office support manager, who will additionally monitor CoSeC usage on ARCHER and report back to the CoSeC manager at regular intervals. A renewal for the CoSeC allocation on ARCHER will be submitted. We will prepare our submission for the 2018 International mid-term review, attend the review and engage with implementing any recommendations that may emerge from this and the Technopolis review.

Support for Drupal based CCP websites will continue and, with support from the CoSeC impact manager, the project office will explore options to increase the impact of the work completed by CoSeC funded projects. The project office will also prepare and submit two reports to the SLA Steering Committee and EPSRC – an annual report covering the full twelve months of the 2017/18 financial year will be submitted in June 2018 and an interim report covering the first six months of the 2017/18 financial year will be submitted in December 2017.

FY 18/19 Staffing	**Effort (FTE)**
Damian Jones	0.70 FTE
~~Viliam Kalavsky~~	~~0.50 FTE~~
Marion O'Sullivan	0.25 FTE
Barbara Montanari	~~0.50~~ 0.25 FTE
RIG Group	0.25 FTE
Total	**~~2.20~~ 1.45 FTE**

Project Office – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Moving forward into 2019/20 the project office will continue with its normal day-to-day activities but will also help to co-ordinate CoSeC involvement in the CCP Review and implement any receommendations made by the panel at the CoSeC international review that takes place in October 2018.

CCP5 – Computer Simulation of Condensed Phases

CCP5 is the Collaborative Computational Project for computer simulation of condensed phase materials at length scales spanning from atomistic to mesoscopic levels. Founded more than 35 years ago, CCP5 has promoted the involvement of UK scientists in collaborative research achieved via software and methodology development, training, networking and outreach. It provides support for all UK scientists engaged in developing, applying and exploiting computer simulation methods for condensed matter systems. CCP5 has over 250 UK members and over 250 international members, which comprise

research active academic faculty staff in 35 different UK universities and at least 18 other UK industrial, charitable or government organisations. A distinctive feature of CCP5 is its successful strategy of developing and disseminating new codes and methods for all kinds of materials problems. These include solid-state materials, polymers, colloidal solutions, liquids and mixtures, liquid crystals, surfaces and interfaces, homogeneous and heterogeneous catalysts, mineral, bio-mineral, organic and bio-molecular systems.

Our core software support covers numerical energy minimisation, classical molecular dynamics and Monte Carlo simulation, ranging from atomistic to multi-scale molecular systems. An increasing effort is exerted to tackle major challenges in cutting edge parallel simulations, linking atomistic and higher level models with first principles (quantum), spanning longer time- and length-scales by means of coarse-graining and mesoscale modelling so as to provide reliable multi-scale simulation protocols.

CCP5 major software and methodology support includes five active projects which together account for over 4,000 active licence holders worldwide in 80 countries. DL_POLY is a general purpose, classical, particle dynamics program. DL_MESO is a general purpose Dissipative Particle Dynamics program. DL_MONTE is a general purpose particle Monte Carlo program. ChemShell is an advanced command line environment with tools and methods for modelling materials systems simultaneously in classical and quantum terms. DL_FIELD is a cheminformatics program for conversion of materials structures from XYZ/PDB description to structure and force-field model files suitable for input into DL_POLY, DL_MESO and DL_MONTE.

CCP5 also provides funding for undergraduate student bursaries, workshop and conference funding and international visitor tours in the UK as well as an extensive range of training events including the annual CCP5 summer school.

CCP5 – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Software Objectives

DL_FIELD is a program to aid the user to setup the empirical potentials employed within DL_POLY. This is complex for large molecules and can often cause errors within the simulation. In the current year DL_FIELD and its underlying database will be extended to allow datasets to be written for Monte Carlo simulations using DL_MONTE, to include the popular MARTINI force field (lipids and some proteins) and to specify more than one potential between the same atom types when ready structures in the xyz format. Once these changes have been implemented a new release of DL_FIELD will occur.

Coarse grained simulations often employ the dissipative particle dynamics (DPD) module within the DL_MESO package. DPD simulations can be enhanced by including electrostatic interactions and the particle-particle-particle mesh (PPPM) method is an efficient method for large simulation cells. This will be implemented within DL_MESO.

CCP5's strategy has identified the requirement for more elaborate force fields for molecular dynamics and Monte Carlo simulations. VS and IS will be responsible for developing a strategy for implementing shaped particles (Gay-Berne potentials) and empirical valence bond potentials respectively. As in previous years updated versions of DL_MONTE and DL_POLY will be released. JAP will also focus on developing the tutorials for DL_MONTE.

ChemShell support under CCP5 will begin to shift from the Tcl version to the Python version following the initial developer release of Python ChemShell. New training materials for the Python-based code will be developed including new tutorials in preparation for future workshops. The website will also be redeveloped. In the meantime, training will continue to focus on the Tcl-based code in this period.

Network Objectives

A significant component of CCP5's activities is focused at training and CCP5 runs a 10 day summer school that introduces first year postgraduates to the methods of molecular simulation. The students undertake 5 days of general theory and then select one of three advanced topics. John Purton is responsible for organising the event alongside a local organiser and this year will take place at Lancaster University. John Purton will lecture and coordinate the afternoon practical sessions and will Michael Seaton co-deliver the "mesoscale" advanced option. As with any course the material requires constant modernisation.

The code developers support users by delivering training workshops in which the core functionality is described. They also help with "user" problems during these surgeries and throughout the year. At least two workshops will be run during 2017/2018.

A new activity for CCP5 is to engage with experimentalist and industrialists. This is achieved mainly by a small conference. During 2017 CoSeC staff will identify a venue and commence the organisation of this event.

Tom Keal is organising the 3rd Joint CCP5/CCPBioSim Multiscale Modelling Conference to be held in Manchester in Q2 2018

CCP5	Milestone	Target Date
	DL_Software @QMUL Complete, 20 participants	Q2 2017
	New release of DL_POLY Complete - postponed slightly due to staff absence	Q4 2017
	Preparation of DL_MONTE workshop tutorials. Complete	Q2 2017
	Release of new versions of DL_MONTE Complete	Q2 2017
	CCP5 Summer School organization & delivery. Delivered a successful event despite staff absence at short notice, 65 participants	Q2/Q3 2017
	For DL_POLY, preliminary investigation of Gay-Berne potentials + strategy plan for implementation Complete, debugging	Q2/Q3 2017
	Advanced mesoscale course at CCP5 Summer School Complete	Q3 2017
	DL_FIELD to create DL_MONTE files. Complete for one FF, awaiting for testing from DL_MONTE team	Ongoing
	Expansion of DL_F notation in DL_FIELD to amino acids Complete	Q1 2018
	For DL_POLY, preliminary investigation of empirical valence bond + strategy plan for implementation Complete	Q3/Q4 2017
	Implementation of PPPM electrostatics in DL_MESO Postponed. Will be started Q3 2018 after the release of DL_MESO version 2.7.	~~Q4 2017~~ Q3 2018
	Improve features for inorganic systems (e.g. freeze) for DL_FIELD Complete	Q4 2017
	Improvement of bio-inorganic system models (e.g. auto mixing of VdW parameters) Complete	Q1 2018

	Identify a venue and date for the "Experimentalist & Industrialists" workshop to be held late 2018 Complete – the workshop will take place in November 2018 at Diamond	Q4 2017
	Prototype of Gay-Berne programs of DL_POLY Ongoing – will move into the plans for 2018/19	Q4 2017
	Training event for ChemShell for CCP5 Complete	Q3 2017
	Hold a DL_Software training event at the University of Strathclyde Complete – 15 attendees	Q3 2017
	Multiple potential capability for DL_FIELD Complete	Q1 2018
	Develop web presence as more interactive – web forms/distro etc In progress	Ongoing
	Redevelop chemshell.org website as a drupal website Complete with user accounts system, forums and software portal all in place.	~~Ongoing~~ Q1 2018

Staffing	**Effort**
John Purton	0.79 FTE
Chin Yong	0.81 FTE
Michael Seaton	0.10 FTE
Thomas Keal	0.08 FTE
Ilian Todorov	0.00 FTE
New Hire	0.60 FTE
Total	**2.38 FTE**

CCP5 – Summary Report (1 April 2017 – 31 March 2018)

The DL_Software and Hack Day events organised at QMUL April 5-7, 2017 were attended by 20 participants.

The three days' splash introduction and training event on DL_MONTE at University of Bath (19-21 April) was a success. The event attracted 25 participants for UK and EU academia.

Dr. Kostya Trachenko at QMUL, started using DL_POLY_4 for his master course in Molecular Simulations. He was also elected as the new executive committee member at CCP5 elections in September.

Drs. Ilian Todorov and Michael Seaton were successful in attracting H2020 funding, awarded in May 2017, for 2 PDRAs over 3 years to work on a software interoperability project, VIMMP, in the area of mesoscale and molecular modelling. The project involves a large number of UE institutions and commercial organisations – industries as well as software houses. On the UK side it includes UNILEVER, IBM UK and University of Manchester.

Prof. Mark Tuckerman from NYU concluded his UK tour as an international CCP5 visitor in May 2017.

CCP5 Summer School was organised for the second year at University of Lancaster, in July 2017 for 10 days and was attended by 67 participants, from all over the world. Dr. Alin Elena took over from Dr. John Purton the running and organisational responsibilities for the school. The school involved not only distinguished academic speakers but also trainers and lecturers from other CoSeC consortia such as HEC-MCC, UKCOMES, CPUK and CCP5.

CCP5 AGM conference organised at University of Strathclyde, 11-13 September, was attended by 87 participants, from UK and overseas, from academia and industry. A DL_Software and Hack Day event, 13-15 September, followed up attracting 15 participants. The executive committee at AGM approved of the choice of Dr. Alin Elena as the acting CCP5 secretary and supported the move to the full role.

The recruitment for the eInfrastructure grant for DL_POLY_4 was successful with Jim Madge being appointed at Daresbury Laboratory (1st of November, from Durham University) and Alex Buccheri at University of Bristol (18th of September, from University of Oxford).

CCP5 Summer Bursaries concluded with a number of 8 students. Reports will be available on the website once all are received.

Prof. Fernardo Escobedo, from Cornell University will be next year CCP5 international visitor, with visits at Cambridge University, Bath and more.

Led by Dr. Ilian Todorov, the organisation of the special meeting to celebrate the DL_POLY projects' 25th anniversary at Chicheley Hall on 3rd November is going to plan. Major stakeholders and power user researchers are confirmed as speakers. The event is sponsored by STFC, CCP5, HEC-MCC, EMCS and Molecular Simulations.

Effort is ongoing on keeping the website up to date and new outreach and impact sections were added.

Molecular Simulation research by Prof. Nora de Leeuw et al. using DL_POLY made the front cover September Issue of Journal of Molecular Chemistry B.

DL_Poly Developers meeting, Darsubry Labs, 6-7 November 2017, 14 participants, with invited speaker from CCP9.

DL_Software training at Daresbury Laboratory, 19-22 February 2018, 27 students attended

CCP5 Summer school 2018 organisation is under way. 88 students have applied for the school, with 48 applying for the programming course. A revamp of lectures and tutorials has been done. Lecturers involved are Prof Neil Allan (Bristol), Dr Paola Carbone (Manchester), Prof John Harding and Dr Colin Freeman (University of Sheffield), Prof Jamshed Anwar (University of Lancaster), Prof Ian Halliday (Sheffield-Hallam University), Dr Michael Seaton (DL, UKCOMES), Prof Stewart Clark (Durham, CCP9 chair), Dr Leonardo Bernasconi (RAL, MCC), Prof Charles Laughton (Nottingham, CCPBiosim), Dr Sarah Harris (Leeds, CCP5Biosim), Dr Christopher Woods (CCPBiosim, Bristol) and Dr Alin Elena (CCP5, DL)

CCP5 Summer School 2019 will happen at University of Durham, with local organisers, Prof Mark Wilson and Dr Mark Miller.

CCP5 –2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

The draft workplans (subject to final approval at the next CCP5 management committee meeting) are as follows:

CCP5 Networking, Training & Outreach: Coordinate and assist part of the organisation process of the two big CCP5 events CCP5 summer school and AGM. Coordinate web presence for CCP5 community (web page, mailing lists). Create a new two days intensive course Introduction to programming for the Summer school. Coordinate the visitors, workshops and bursaries programs of

CCP5. Collate data for various reporting milestones for CCP5 and CoSeC. Update CCP5SS practical exercises material and assist the sessions. Assist practical tutorials at the AGM and coordinate events as Nuclear Materials Modelling and Outreach to Experimentalist and Industrialists. Coordinate and deliver DL_Software training workshops. Update website infrastructure with new materials and sections.

DL_MESO: Following the release of version 2.7, CCP5 effort on DL_MESO development will concentrate on expanding the range of systems that can be modelled using dissipative particle dynamics: in particular, fixed-length constraints will be implemented to allow larger timesteps to be used when modelling molecules. A new set of lattice Boltzmann tutorials based on DL_MESO will be developed (in collaboration with Ian Halliday at Sheffield Hallam University) for the CCP5 Summer School's advanced mesoscale course.

DL_POLY: With the parallel development of two new major strands of DL_POLY, Empirical Valence Bond (EVB) and Shaped Particles (SHP) as well as the start of flagship developments of Density Functional Tight Binding (DFTB) and Forward Flux Sampling (FFS), the project is in a critical need to undergo an extensive refactoring before prototype projects can merge and develop further. The refactoring work will include mapping, new coverage test cases, performance scaling recording, new user relevant and EVB and SHP project webpages.

DL_MONTE: The project has been actively developed over the last three years. With a number of parallel developments it needs extensive testing, extension of the library of user cases and a large amount of code clearing up. This work will be undertaken in two stages (i) library of user test cases to demonstrate functionality, (ii) extensive testing. JAP will also supervise and coordinate the project effort coming from external partners at the University of Bath.

ChemShell: Following the initial release of the redeveloped Py-ChemShell code, ChemShell CCP5 effort will be reoriented towards Py-ChemShell. A new full set of training presentations and hands-on tutorials will be developed for the Py-ChemShell code for use in DL_SOFTWARE training workshops, where both Tcl-ChemShell and Py-ChemShell will be taught until Py-ChemShell fully supersedes the legacy code. Support for Py-ChemShell file formats will be introduced into the Aten GUI via a plugin. A regular schedule of releases of Py-ChemShell will be maintained.

DL_FIELD: The software continues to develop at multiple fronts, both organic and inorganic force fields (FF) and mixture of both. New FFs will be introduced including zeolites, MOFs, Amber Gaff, Charmm DNA and ionic liquids. Some form of automation is now possible for bio-inorganic model set-up, especially for clay+organic materials. More new bio-inorganic features will be included and further expand, especially the automation setup procedure for other types of inorganic materials.

DL_ANALYSER: The unique capability of the software to detect and quantify various modes of localised atomic interactions by making use of the DANAI expression has been released. Such features will be further developed to include other types of interactions including H-bond interactions, aromatic pi-pi interactions and charged-dipole interactions.

FY 18/19 Staffing	**Effort**
John Purton	~~0.79~~ 0.45 FTE
Chin Yong	~~0.31~~ 0.51 FTE
Michael Seaton	0.10 FTE
You Lu	0.20 FTE
Vlad Sokhan	1.00 FTE
Ivan Scivetti	1.00 FTE
~~Ilian Todorov~~ Alin Elena	~~0.00~~ 0.68 FTE
Total	**~~3.40~~ 3.94 FTE**

CCP5 – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

CCP5 Summer School moves to University of Durham, organize with the transition. Organise a cross community effort about forcefield parametrisation, initially CCP9/CCP5Biosim and ISIS.

To provide more scalable electrostatic interaction calculations with local polarizability effects, the Groot DPD electrostatics scheme based on the particle-particle particle-mesh (PPPM) algorithm will be implemented in DL_MESO. DL_FIELD support for xyz for inorganic models by further expending DL_F notation to inorganic models. New refactorised DL_POLY with fully modular structure. Chemshell will develop further the interface to DL_POLY_4 to target the refactored code and improve the Aten plugin for gui.

CCP9 – Electronic Structure of Solids

The Collaborative Computational Project on Computational Electronic Structure of Condensed Matter (CCP9) brings together UK researchers in the field of ab-initio electronic structure calculations of condensed matter systems. The field includes the study of metals, semiconductors, magnets, and superconductors from atomistic quantum mechanical calculations. The activities of CCP9 encompass such areas as magneto-electronics, photonics, nanotechnology, high-temperature superconductors, novel wide band gap semiconductors, and magneto-calorics. CCP9 provides a network that connects UK research groups in electronic structure, facilitates UK participation in the larger European Ψk Network, and is supporting a number of cutting edge computational codes.

CCP9 – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

CCP9 novel materials support is focused on correlated electron systems and magnetism. Especially with respect to the latter, there is an ongoing collaboration with Julie Staunton at Warwick University using the KKR-DLM code to study on magneto-calorics (Gd-intermetallics) and permanent magnets (GdCo5). A recently established collaboration with Laszlo Szunyogh at Budapest University aims to investigate on ab-initio magnetism in Mn3Sn. A further area of research deals with the electronic structure of nuclear materials.

Validation and verification: After successfully demonstrating the accuracy of the CCP9 flagship code QUESTAAL with respect to the elemental solids, the next step will involve extending the study to the rare-earth elements, and comparing the results to those from pseudopotential calculations through collaboration with the CASTEP team.

Implementing and testing of the self-interaction correction into the QUESTAAL code: Work is currently ongoing to determine how best to implement the SIC formalism into the full potential code. The aim is among others to be able to compute valence and structural transformation in correlated systems from first principles. A further QUESTAAL code development aims to enable the calculation of crystal-field parameters, in collaboration with Mark Hughes at Salford University.

CCP9	Milestone	Target Date
	Collaboration with Julie Staunton on permanent magnet materials, visit and discussion Ongoing. This collaboration has produced one publication so far this year.	ongoing
	Workshop: LMF-QSGW hands-on course Complete. Very successful event with thirty attendees.	Q2 2017
	V&V for the elements (if successful project will extend to lanthanides, Q3 2017) Complete. Upload to DeltaCodes server expected March or April 2018, pending approval by principle code developer. New basis	Q2 2017

	setup algorithm developed and implemented which significantly improves FP-LMTO method reliability/accuracy. Jerome is planning to write a paper summarizing the results.	
	Deliver capability to evaluate CF parameters in LMF (collaboration) Ongoing. Jerome and Mark Hughes have submitted a proposal to EPSRC for funding. They have requested three months of Jerome's time to complete the work via a responsive node grant. The grant has been accepted, and intial planning meeting has taken place. Awaiting discussions with Mark Hughes and Stanko Tomic. Will move into 2018/19 plans	~~Q2 2017~~ Q4 2018
	Organize CCP9 working group meeting Complete. The recent Young Researchers event organised with Mike Payne included a working group meeting. Looking to reorganise the working group going forward following Mike Payne's resignation. A new chairman is now being sought.	Q2 2017
	Implementation of SIC in LMF; initial phase Complete	Q2 2017
	Flexible atomic solver in FPLMTO, technical report Complete. The work is done. Jerome will be writing up and producing the report.	Q3 2017
	Submit results on Ab initio magnetism of Mn3Sn (collaboration) Ongoing. Paper draft received from experimental collaborators (Seoul), currently in discussion with theoretical collaborators (Budapest team). Will move into 2018/19 plans.	~~Q3 2017~~ Q3 2018
	Results on TM-oxides Ongoing. Further tests required concerning the comparison of different codes. Delayed due to other more relevant tasks. Will move into 2018/19 plans.	Q4 2017
	Publish article on magnetism in Gd-alloys Ongoing. The calculations are done. The paper is in the process of writing up	~~Q4 2017~~ Q3 2018
	Results magnetic properties of GdCo5 Complete. The work is now published	Q4 2017
	Workshop: KKR hands-on course Ongoing. Combined experiment (SuperSTEM) theory workshop is planned for June 2018	~~Q1 2018~~ Q2 2018
	Submit Rare earth doped ceria article Ongoing but delayed because of other work.	~~Q1 2018~~ Q4 2018
	Workshop on atomistic simulations of nuclear materials Planned to be a combined CCP5/CCP9 workshop, it will be organized in Bristol in June 2018	~~Q1 2018~~ Q2 2018
	Implementation of SIC in LMF; demonstration Ongoing pending further consideration.	~~Q1 2018~~ Q3 2018

Staffing	**Effort Funded**
Leon Petit	1.00 FTE
Martin Lueders	0.20 FTE
Jerome Jackson	1.00 FTE
Total	**2.20 FTE**

CCP9 – Summary Report (1 April 2017 – 31 March 2018)

Support for the Flagship Project: The CCP9 flagship code "Questaal", apart from density functional theory (DFT), also implements GW, a Green's function based approach, in both its one-shot and self-consistent forms, enabling the incorporation of many-body effects and the calculation of among others improved semiconductor band-gaps and excitation spectra. The validation and verification project, where the accuracy of the full potential lmf code (part of Questaal) has been systematically compared with that of other all-electron and pseudopotential DFT implementations, has resulted in a set of highly accurate data for the elements and that will be shortly uploaded to the Δ-Codes project website. A report on the accuracy of different core boundary conditions in the lmf code was finalized by Jerome Jackson. With respect to parallelization of the QSGW, the collective IO in HDF5 has been fixed by Martin Lueders. Calculations for systems with up to 80 atoms are ongoing. A Questaal hands-on course was organized May 16-19 at Daresbury Laboratory. Martin Lueders and Jerome Jackson presented their work at the Questaal steering committee meeting at KCL.

Research on correlated electron systems: Leon Petit has been involved in a theory-experiment collaboration with Warwick University, investigating the intrinsic magnetic properties of the compounds YCo5 and GdCo5. The goal of this collaboration is the probe the interactions that govern the rare-earth/transition-metal permanent magnets and to study the corresponding magnetic ordering temperatures. The results of this study have recently been published [Phys. Rev. Mat. 1, 02441 (2017)] and [Phys. Rev. Lett. 120, 097202 (2018)]. Work on Fe3O4, and NiFe2O4 is currently ongoing. In connection with the collaboration on magneto-caloric materials with Warwick University and Ames Laboratory (US), an article on Gd-intermetallics has been published in Magnetism and Magnetic Materials [J. Magn. Magn. Mater. 448, 9 (2018)].

CCP9 Young Researcher Event and Community Meeting: The event was held at Clare College, Cambridge, 10-11 April 2017, with altogether 95 participants.

Crystal-field parameters in lmf: The EPSRC proposal titled "Rare-earth implanted silicon for solid-state quantum technologies" by Mark Hughes (Salford University) PI, and with Jerome Jackson as co-investigator has been approved. Initial theory results on the lattice relaxation in connection with doping Er into silicon have been discussed with the collaborators at Salford University.

A proposal on modelling EELS spectra using Questaal has successfully passed the SCD internal Bid review, and is about to be submitted to EPSRC. The collaboration involves the SCD (Jerome Jackson who is PI on this project and Leon Petit) as well as SuperSTEM at DL, and the universities of Leeds, York, and Belfast.

Psi-k: CCP9 provides support for the European electronic structure network Psi-k in the form of finance administration and editing the Psi-k scientific highlight. Five highlights were edited during the reporting period, and submitted to the mailing-list which now reaches more than 3500 people.

CCP9 – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

CCP9 novel materials support is focussed on correlated electron systems and magnetism. Especially with respect to the latter, there is an ongoing collaboration with Julie Staunton at Warwick University using the KKR-DLM code to study the properties of magneto-calorics (Gd-intermetallics) and permanent magnets (GdCo5). A further collaboration with Laszlo Szunyogh at Budapest University aims to investigate on ab-initio magnetism in Mn3Sn.

Code development: Questaal is the current CCP9 flagship, with the goal to produce a new community code for electronic structure. A main effort from DL deals with implementing and testing the self-interaction correction into the code. The aim is among others to be able to valence and structural transformation in correlated systems from first principles. A further Questaal code development aims to enable the calculation of crystal-field parameters. The project results from a successful joint EPSRC

proposal with PI Mark Hughes at Salford University. Other code development will be in connection with the parallelization of CRYSTAL and the update of DLV.

Novel opportunities: Submitting a proposal with collaborators at SuperSTEM Daresbury, and the universities of York and Leeds to improve our understanding of fundamental physics in STEM experiments through modelling from first principles.

Staffing	Effort Funded
Leon Petit	1.00 FTE
Martin Lueders	0.26 FTE
Jerome Jackson	1.00 FTE
Barry Searle	0.60 FTE
Total	**2.86 FTE**

CCP9 – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Assuming the STEM proposal is successful, a postdoctoral research assistant will be hired to work on the project in collaboration with people at SuperSTEM as well as York, Belfast, and Leeds Universities. A new group leader will be in charge of the TCPG, and future plans also for CCP9 will have to be discussed with her/him.

CCP-mag – Computational Multiscale Magnetism

Magnetism and its microscopic understanding are of high importance in a number of vital technologies, starting from the energy sector, such as permanent magnets in the generators, to computer technology, for instance magnetic RAM, hard drive technology. Modelling magnetic properties can speed up the process of developing novel materials for these applications.

The UK has mature communities in magnetic modelling at various length scales, as well as a strong experimental community, mainly around the ISIS neutron scattering facilities at Rutherford Appleton Laboratory (RAL). This embraces simulations on different length scales, starting from ab initio calculations of magnetic properties (based on the full quantum mechanical description), over atomistic modelling, representing magnetic materials by spin models, up to micromagnetics, utilising finite element techniques to describe larger systems or whole devices.

The Collaborative Computational Project on Computational Magnetism was established in 2015 to bring researchers from these communities together and make the expertise of ab initio electronic structure codes, partially developed within the CCP9 community) available to them.

CCP-mag – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

The main part of the work is concerned with implementing a common data format, through which data produced by ab initio calculations can be easily and routinely imported into atomistic spin modelling codes. This task will be done in collaboration with the CECAM Electronic Structure Library activity. Besides that, the core support team will coordinate the activities of the corresponding networking grant, which includes the organization of Hands-On courses and the coordination of conferences. In agreement with the CCP-mag Chair, the amount of effort planned for FY 17/18 is below average and this will be compensated by an above average effort in following years.

CCP-mag	Milestone	Target Date
	NMAG installation procedure This activity is no longer necessary as it is no longer of interest to the community	Q2 2017
	Co-ordinate session at IOP Magnetism 2017	Q2 2017

	Complete. A working group meeting was held during the conference. Also had an OOMF conference where the developer attended. Martin was on the organising panel for the conference	
	Finalize data structure for geometry Complete. The data structure is documented on the ESCDF web pages.	Q3 2017
	Finalize data structure for exchange couplings and anisotropies Paused, as the new design of the library will make extensions, such as magnetic couplings trivial.	Q3 2017
	Implementation of basic infrastructure of ESCDF library The design of the library has changed to make it easier to extend it in future. The new implementation is currently in testing phase.	Q4 2017
	Run KKR course (joint with CCP9) Postponed. A new date will be discussed.	Q1 2018
	Continued support for ISIS Work on Fe has been completed and a publication is planned. The work was well received at a conference in South Korea. A second project on Ni is being considered, as well ad full 4D data calculations.	ongoing

Staffing	**Effort**
Martin Lueders	0.25 FTE
Barry Searle	0.15 FTE
Total	**0.40 FTE**

CCP-mag – Summary Report (1 April 2017 – 31 March 2018)

During the reporting period, the core support was operating at reduced effort of 0.4 FTE as we concentrate the available resources towards the last two years. in February, Dr. Kun Cao was hired and is employed full time on this project. He will work on higher order exchange couplings and also on the magnetic excitations project with the facilities.

As part of the common data format project, Yann Pouillon and Micael Oliveira, the main developers of the CECAM electronic structure common data format (ESCDF) library visited Daresbury for one week to work with Martin Lueders and Barry Searle on the implementation. These visits were funded externally through the COST network EUSpec. During this week, the part of the standard and library which deals with the geometry of the system (lattice parameters, position of atoms, etc.) has been finalized and is currently being tested.

The library development has been continued during a CECAM ESL coding workshop in Lausanne in February and a visit to Micael Oliveira, where it was decided to change the design of the library to make it more easy to maintain and extend in future. This new design has been presented at a EUSpec meeting in Lisbon at the end of February. The implementation of the new design is mostly finished and currently in the testing phase.

Good progress has been made on the spin excitation project with ISIS, which is partially funded through direct funding from the STFC facilities programme. Test calculations performed with the KKR code and the QUESTAAL code package showed extremely good agreement, despite using very different methodologies. This gives assurance that both codes are reliable. Toby Perring (ISIS) presented first results at a neutron scattering conference in South Korea and had very positive feedback. Calculations of the whole 4D data set (full Brillouin zone and frequency range) are ongoing.

The full 4D calculations for iron have been completed and a paper is in preparation. Martin Lueders will present the results at the IoP Magnetism conference in Manchester on the 9th of April.

CCP-mag – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

In the period 2018/19 we will continue the programme of workshops, hands-on courses and support of the IOP Magnetism conference. It is planned to further develop the ESCDF library, and in particular, add the data fields relevant for the magnetism community.

As the new recruit for the CCP core support will be in place, we can now put more efforts into the investigation of ab initio calculations of exchange couplings, including a detailed comparison of existing methods, and also the development of new methods going beyond this by including higher order terms and non-collinear spin structures.

The support for ISIS, which also generated external direct funding from the ISIS neutron scattering facilities, will continue and we will investigate methods beyond the so-called rigid spin approximation.

Staffing	**Effort**
Martin Lueders	~~0.25~~ 0.22 FTE
~~Barry Searle~~ Kun Cao	~~0.15~~ 1.00 FTE
Total	**~~0.40~~ 1.22 FTE**

CCPmag – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

In the period 2019/20 we will continue the programme of workshops, hands-on courses and support of the IOP Magnetism conference. The ESCDF library should then be ready to be rolled out to community codes, and we plan to interface an ab initio electronic structure code via the library with the VAMPIRE code. We plan to finish the implementation of higher order exchange couplings.

The support for ISIS will continue and we will investigate methods beyond the so-called rigid spin approximation and in particular beyond density functional theory, using QSGW + DMFT.

CCPNC – NMR Crystallography

Nuclear Magnetic Resonance (NMR) is a useful technique to determine chemical structure, especially in compounds of which it is hard to produce single crystals big enough for diffraction techniques, as commonly found in organic molecules. NMR Crystallography is the technique of using quantum-mechanical simulations to predict NMR spectra to a high degree of precision, and combining this with experiment to open new ways of exploring structure in not yet understood crystals, such as new pharmaceuticals. CCP-NC has the objective of disseminating and promoting this approach throughout the experimental NMR community in the UK and worldwide.

CCPNC – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

During the coming year, the CCP-NC will focus on maintaining the high level of support for the tools and practices it promotes across the community as well as increase the ability of experimental NMR groups to make use of computation in their work. This objective will be pursued by multiple approaches.

Firstly, through communication and ground testing, a protocol will be established for the storage and classification of existing NMR computational results, as a necessary step towards the development of a shared database. The database itself will be prototyped and user feedback will be gathered in view of a public deployment. Secondly, Soprano (a library for the analysis of computational data sets) will be further developed in response to the specific needs of the community. The Tran-Blaha exchange-

correlation functional, a needed improvement to the CASTEP ab-initio software with regards to the precision of NMR calculations involving certain critical nuclei such as fluorine, will be tested and deployed. New requested functionalities will be added to MagresView, particularly to ease the interfacing with external software. Finally, the ties with the muon spectroscopy community will be developed further and any chances to reuse existing techniques and software and develop connections between the methods used in either field will be pursued.

CCP-NC	Milestone	Target Date
	Upgrade and maintenance of the CCP-NC website and its content (SS, AB) Website is now complete, available live and being updated.	Ongoing
	MagresView code maintenance and extension (SS) Maintenance is ongoing. No new major features or reparsing are scheduled at the moment.	Ongoing
	Development of a prototype of an NMR database (AB) Complete. A full first version of the database front-end is available for testing by the community, and all final functionality is present in its basic form.	Q2 2017
	Integration of MagresView with said database (SS) Postponed until the community gives final approval on the current format adopted by the database, and will be prioritised afterwards against other tasks depending on which are considered the most pressing needs.	~~Q2 2017~~ Q1 2019
	Writing and submission of a paper on new approaches and techniques for the interpretation of muon spectroscopy results using ab-initio calculations and including complex effects (quantum tunnelling, temperature dependence, phonons) (SS) Paper has been published in Q1 2018 and is now online.	Q3 2017
	Moving Soprano from alpha to beta stage (SS) Complete.	Q4 2017
	Inclusion in CASTEP of the Tran-Blaha functional (AB) Fully functional and a paper is currently being written up. Plans for release, but depending on other similar functionality.	Q4 2017
	Release with CASTEP of the NICS tool (SS) In progress. It is ready and will be discussed with the next release of CASTEP	~~Q4 2017~~ Q4 2018
	Writing and submission of a paper on the topic of the Lorentz sphere and the range-dependent relationship between current fields and chemical shieldings in crystals (SS) Theoretical framework and software are complete, but the paper's writing has been postponed due to the higher priority of other tasks	~~Q1 2018~~ Q1 2019
	Testing and assessment of the feasibility of machine-learning techniques with regards to NMR parameter prediction, esp. in organic molecular crystals (AB) Progress in adapting a simple Tight-Binding model to predict the NICS of aromatic hydrocarbons, and integrating it with machine learning.	Q1 2018
	Development of scripts and tools to encourage use of Soprano within the muon spectroscopy community Ongoing. A repository of private scripts is available and specially developed Jupyter notebooks have been used in the ISIS Muon school's tutorials. New functionality dedicated to this purpose has been added to Soprano too (interstitial defect generation). This activity will continue depending on our interactions with the muon community and any emerging needs.	~~Q1 2018~~ Q4 2018

Staffing	Effort Funded
Simone Sturniolo	1.00 FTE
Albert Bartok-Partay	1.00 FTE
Total	**2.00 FTE**

CCPNC – Summary Report (1 April 2017 – 30 September 2017)

The Soprano Python library, developed by SS and aimed at helping crystallographic searches, has been upgraded with more NMR related functionality and the use of bond order parameters, especially useful for analysis of defects and disordered structures. Version 0.7.1 has been officially released, including the new functionality for the generation of random interstitial defect structures, and the library has been tested in a number of practical applications, including a successful test search for muon sites in diamond-like structures which will be part of a soon to be submitted publication.

Development of a CCP-NC Magres files database has been going on steadily. A full prototype for the final application is now available, using ORCID as an authentication system to guarantee the identity of uploaders, and providing functionality for uploading, searching, downloading, and editing entries, tracking multiple versions for each record.

A new CCP-NC website has been developed based on a modern and well-supported content management system, Grav, to be easier to maintain and update. The new webpage allows viewing on a range of devices, easy editing, as well as new features, such as webforms. The latter was used to manage the CCPNC bursary applications and user registration for the CCPNC-provided HPC access.

CCP-NC is now providing access to High Performance Computing for its members via the UK Car-Parrinello Consortium. Having joined the UKCP, CCP-NC is given an allocation on the newly commissioned Thomas machine in UCL, allowing CCPNC users to submit large calculations, try new functionality or receive support on problematic tasks. CCPNC manages its own group on Thomas, providing its users with software tools and data sharing. With ten CCP-NC users already, some of whom having no other means to access high-performance computing facilities, this new opportunity has proved to be highly successful.

ABP continued his work on implementing new functionality - in particular, meta-GGA type exchange-correlation functionals - in CASTEP, and he presented preliminary results at the annual UKCP meeting in July. The new capabilities of the code were also benchmarked by a summer student and a postgraduate student in the Materials Department in Oxford in the contexts of NMR parameter prediction and band structure calculations. Details of the implementation are of general interest, and a publication is currently in preparation. Development of new types of density functionals is a very active field, promising significant improvements, and work to incorporate these in CASTEP has progressed further, for example implementing the new SCAN functional.

In collaboration with Abil Aliev, a solid-state NMR researcher in UCL, ABP performed calculations that helped to interpret the spectra of tin-oxide compounds, and a paper reporting the results has recently been published in Solid State Nuclear Magnetic Resonance.

CCPNC – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

For the 2018/19 period, the work will focus on maintenance and development of currently ongoing software projects, as well as exploration of both new tools and solutions and pursuit of a better

understanding of the way NMR parameters emerge from crystal structure, with the aim of providing a more solid theoretical basis, as well as infrastructure, to the NMR crystallography community.

A first version for an official CCP-NC database to store calculation results is already in place on a permanent STFC server, with a basic schema for data storage. Through 2018 and 2019 we plan to put in place security and data backup infrastructure, establish a policy on licensing for the uploaded data, and reach the stage where it can be deployed to the public for day to day use. The database follows the model of similar efforts in crystallography like the OCD; for authentication it currently relies on the ORCID public API.

A continuous effort for maintenance and improvement of Soprano is ongoing. More so, it will be key to disseminate information about it to the community through conferences, workshops, private collaborations, and online presence. This will concern both the NMR and the muon spectroscopy community, which is manifesting an interest in the library as well. A first paper about work using the library has been published, and the objective will be to produce more.

Since the original development of MagresView, the Javascript ecosystem has undergone great leaps forward, with more tools now available than ever. Reframed as a modern Javascript application that takes full advantage of these tools, MagresView has the potential to become more performant, more compact, more compatible across browsers and devices and overall easier to maintain. It is therefore desirable to implement these changes, that however would require a longer effort than ordinary maintenance, to bring up a radically new version of MagresView.

Computing NMR parameters with DFT does not simply allow us to predict experimental results for known system, but also investigate how the magnetic fields originate in the first place, and understand better the physics which connect crystal structure and NMR properties. A project has been ongoing to use these insight to better define the concept of a ‘Lorentz sphere’, the volume or scale on which local effects are relevant to chemical shifts. This has resulted in a solid theoretical description of the way shielding contributions build up through space. We plan to write and submit a paper reporting our findings next year.

A common issue when interpreting spin resonance experiments for light nuclei and muons is that of quantum effects, and how they tend to add a correction to the classical results given by CASTEP. In order to refine the interpretation of experiments, better, more efficient methods of including nuclear quantum effects are key. The Many Interacting Worlds approach has been under development for a while now and it shows potential promise in treating these issues. It will be developed further and tested on simple system to assess the feasibility of its use. A paper on the fundamental theory has been submitted and reviewed by PRE and is currently undergoing major revisions.

With improved, meta-generalised gradient functionals soon available in CASTEP, extensive testing of this new methodology will began, focussing on the accuracy of NMR parameter prediction. Another important aspect will be assessing the quality of structural parameters, and it is foreseen that dispersion corrections will be needed for some classes of systems, for example, molecular crystals. It will be explored whether the currently used dispersion parameters may need adjustment.

Machine learning potentials can be used to generate structures of materials much faster, without the need to run DFT - for NMR calculations structures being the input, these can speed up the process considerably. Various aspects of machine learning applications are currently planned:

1) Fitting NMR parameters
2) In conjunction with 1), building a long-range interaction model for NMR shieldings These models will allow estimation of NMR parameters without running an electronic structure calculation, accelerating high-throughput applications.

3) Generating a machine learning model for electrostatics parameters, including charge transfer
4) In conjunction with 3), creating a machine learning potential framework which can be used to model molecular crystalline materials

Staffing	Effort Funded
Simone Sturniolo	1.00 FTE
Albert Bartok-Partay	1.00 FTE
Total	**2.00 FTE**

CCPNC – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

By 2019, we plan for the CCP-NC database service to be available to the public and fully functional. It will therefore be possible to undertake projects that make use of it, as well as re-direct effort towards developing other software. One avenue that can be pursued is the automation of a pipeline that computes NMR parameters for known crystalline structures in existing databases and uploads them to the CCP-NC one. There are also plans to rewrite MagresView into an updated 2.0 version which would make full use of the modern HTML5 and JavaScript ecosystem to provide a more maintainable code and better performance. Finally, the new opportunities opened by the implementation of SCAN in combination with dispersion correction schemes in CASTEP will require extensive testing and exploration, and may open up spaces for new collaborations.

CCPQ – Quantum Dynamics in Atomic Molecular and Optical Physics

The remit of CCPQ is to develop code for quantum dynamics simulations, solving the time-dependent Schrödinger equation for both heavy (nuclei) and light (electrons) particles. It has 3 main community codes covering different areas

- *TNT: A package coding Tensor Network Theory for coherent many-body nuclear dynamics*
- *R-Matrix Suite: A set of programs for electron (positron) -atom and -molecule scattering, (ultrafast) laser pulse interactions and related problems*
- *Quantics: A package based on the MCTDH algorithm for molecular quantum dynamics*

The collaboration also has related code development in the field of coherent dynamics in the CCE (Cluster Correlation Expansion) code and in the field of anti-matter scattering related to the R-Matrix work. It also supports codes and research in low-energy antimatter interactions (positron and antihydrogen collisions with atoms and molecules)..

CCPQ – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Core support for CCPQ can be divided into three main types: detailed scientific and computational collaborative research and code development/optimization, more general best practice software engineering and 'continuous integration' support, and general administration including the CCPQ website. The first type is concentrated in the electron collisions, multiphoton interactions and antimatter areas. This will continue in 2017-2018 given the success of the Flagship proposal in the 'R-matrix' collisions/multiphoton areas, to develop and unite the 'RMT' (atomic electrons responding to and ionizing in laser pulses) and 'UKRMol+' (electron/positron-molecule low-energy collisions, excitation and resonance formation) code packages. The R-matrix method effectively solves the time-independent and the time-dependent Schrödinger equation directly for many-electron systems, making use of separate appropriate ab initio treatments for different regions of configuration space, namely the 'inner' region containing the 'target' atom or molecule, and 'outer' regions away from the target containing 1 or, recently, 2 electrons (or positrons).

Martin Plummer is involved several areas, including development of a 'double-continuum' electron-atom theory and code: 2 electrons are treated as ionizing and long-range, rather than 1 as in standard theory,

allowing much more realistic treatment of inner-shell excitation and ionization, and thus (e.g.) high harmonic generation, coherent control of electronic state evolution and understanding of complex transitions and spectra. We note that planned relativistic developments of the atomic code will now be carried out by a PDRA thanks to a separate successful EPSRC grant application by QUB. Andy Sunderland is mainly involved with optimization and parallel development of the UKRMol+ package, as well as porting and optimization to novel architectures. SEG provides support across the range of application areas and groups and runs the Software Engineering Support Centre (SESC), thus providing advice on improving general coding standards, achieving longevity, management of code development and user-friendly running via scripts, assisting with use of their continuous integration tool the 'SESC Build Service' (SBS), and maintaining codes on the CCPForge platform. As well as the R-matrix codes, the SEG support covers the QUANTICS reactive molecular scattering code, for which they will also provide some load-balancing optimization for the parallel code, and the strongly correlated systems code package TNT (Tensor Network Theory) developed at Oxford and Bath (also the UCL package CCE: 'cluster correlation expansion'). General administration is provided by Damian Jones and the SCD Impact manager, with CCPQ-specific support (website content, steering panel minutes etc) by Martin Plummer.

CCPQ	Milestone	Target Date
Atomic R-matrix	MP to receive co-author comments and then referee comments on the theory paper. Continued coding of many-electron double-continuum code and commence detailed testing against QUB independent (restricted) 3-electron code. Initial discussions with QUB as to whether MP should concentrate additional support on the Flagship RMT objectives or consider support as required for the separate new 'relativistic extensions' PDRA. Flagship Discussions (at end of October) concluded that MP should concentrate fully on optimization and various test/initial applications of the double-continuum code: the QUB PDRAs for the Flagship and the relativistic projects are very good. The d-c work is very important and MP's work will maintain its momentum. Thus theory and computational double-continuum work is now ongoing (into 2018-9) following summer support for HEC proposal (see below). MP (and DJ) to support the attosecond science seminar series as required, and to discuss preliminary requirements for the large 2018 international Attosecond Science Workshop (UCL). Attosecond Set-up and registration site COMPLETE. DJ and MP are available for further work should the conference organizer (Agapi E., UCL) require further work.	Q2-Q3 2017 Q4-Q1 2018 and into 2018-2019
UKRMol+	AGS to implement next stage of UKRmol+ memory optimization (from his algorithmic development approved by JD Gorfinkiel (OU) and Z Masin (MBI Berlin) in Q1), commence write-up of this (eventually to form part of a paper with JDG and ZM) and work as necessary with eCSE PDRA A Al-Rafaie on compatibility with the UKRMol+ diagonalization module. MP to maintain contact with AAl-R over parallelization/shared-memory-segment work. Ongoing. final testing and write-up underway. The work was presented at the Flagship meeting to acclaim. A further extension and new indexing transformation algorithms for this upgrade was agreed at the meeting and AGS is to concentrate on this for Q4-Q1: substantial memory gains achieved (eg 4Mbytes -> 29 kBytes for one array modules in a test case)	~~Q2 2017~~ Q3 2017 Q1 2018

Novel Technology/ PFARM	AGS to supervise/produce 'accelerator' versions of PFARM (EXDIG stage) which are designed for GPU and Xeon Phi architectures [(1) Modern GPUs (e.g. K20 onwards); (2) Knight's Corner Xeon Phi; (3) Knight's Landing Xeon Phi] for general use and to be part of the PRACE Unified European Application Benchmark Suite (to enable benchmarking of new architectures representing a wide range of scientific fields). This work is in collaboration with DL's PRACE 4 effort (and complements ICHEC collaborator M Lysaght's work on the EXAS stage of PFARM). Complete. PFARM is now part of the European Accelerator Benchmark Suite. A write-up is available as a PRACE deliverable report on the PRACE website	Q2 2017
Novel Technology/ PFARM	Ideally (if time allows), MP and AGS to further support novel/heterogeneous technology adaptations and maintain PFARM's lead in this (through further PRACE applications etc): also dependent on collaborator M Lysaght's work timetable at ICHEC and availability. Ongoing – M Lysaght has left ICHEC to join a bank. No replacement in place for this code.	Q2 2017 and onward
QUANTICS	Quantics meeting at UCL (SEG, MP) to decide on SL's support following return from sick leave (at the time of writing, this meeting has taken place, see below for milestones). Complete	Q2 2017
TNT	DJ to set up webpage for online payment for 'Windsor 2017' cold atoms /strongly-correlated-systems workshop. Complete	Q2 2017
TNT	To be led by SEG following Stephen Lamerton's return from sick leave, consultation with Oxford/Bath (and UCL) to review TNT (and CCE) support needs (SEG, MP AGS). Consultation with Oxford PDRA M Lubasch COMPLETE: prioritize Python Interface in Q3-Q4 If appropriate: upgraded TNT Python interface work (SL). Plans for joining SESC Build Service (SL). Ongoing. SL will be leaving SCD in January: his priority is to hand over management of the Build Service. For CCPQ he has introduced ML to Alan Kyffin (SESC/SEG) who will take over the Python work once he comes back from parental leave (SEG is short-staffed due to paternal and maternal leave at the moment: CJ will formalise SL's full replacement in due course.	Q2 2017- Q3 2017
Antimatter	MP to meet and commence support for MM Law's (year 1) PhD student at Aberdeen (advice or more practical as required). Postponed by Aberdeen until Q3 at their request.	~~Q2 2017~~ Q3 2017
General	General website support and encouragement of member-led submissions, support for workshops. Support for funding applications as they arise. Implement new page listing/linking CCPQ (related) publications. Ongoing. Important funding application with the HEC proposal (PI JT, co-Is HWvdH, JDG): New HEC for R-Matrix application. Core support help with details of the proposal (software and software development plans). MP is on the management group, and	Q2 2017- Q4 2017 (publications list set-up), general support continuous

	specific CoSeC support is requested. HEC proposal complete. Note: the proposal was successful. Publication list to be set up Q4 into Q1: COMPLETE.	
QUANTICS	Adapt Quantics current manual build and subsequent test suite runs into the SESC Build Service for automated execution as standard (SL, as decided at Q2 meeting). Complete	Q3 2017
Flagship (Atomic R-matrix and UKRMol+)	Project meeting (PI H van der Hart, QUB, co-I JDG) with both PDRAs in place, planned for mid-September. Plan for SEG project support to be devised. Plan for new core support work by MP and AGS specifically related to the Flagship to be decided. (cf above discussions with QUB, for UKRMol+ possible support could include AGS assistance with: optimization of dipole transition moments coding AND/OR the interfacing routines that turn UKRmol+ output into RMT input). Meeting held in October. MP to concentrate on d-c work. A range of options for AGS put forward (see plans for 2018-2019) to complement work by the OU PDRA (who has not yet been appointed: the PDRA was appointed in Q1 2018).	Q3 2017
NEW: RMATREACT	PFARM to be adapted to heavy particle collisions as part of the new RMAT_REACT ultracold chemistry project (UCL) whose main development work is planned as part of HEC proposal (or future eCSE/CoSeC effort). MP adapted code and completed initial test case: COMPLETE. Follow-up tests provided for Q4 and further development to be agreed for Q1. : a fuller range of more general interatomic potentials has been included (this stage COMPLETE).	Q3 2017 (into Q4 possibly Q1 2018)
UKRMol+	DJ to support (via web bookings) the planned Quantemol UKRMol+ training day as required Complete. Workshop took place with basic web-advertising from us.	Q3 2017
UKRMol+	Ongoing support for UKRmol+ optimization (AGS): complete technical write-up of memory optimization, commence work on symmetry adaptation of atomic orbitals into block diagonal molecular type orbitals (fairly substantial task). Ongoing. This task is moving into Q4 – Q1 (see above) with extended optimization: now effectively complete, write-up underway, waiting for feedback from collaborators.	~~Q3 2017 - Q4 2017~~ Q1 2018
Atomic R-matrix	MP to agree with HvdH worthwhile cases for initial new work with double continuum code (as opposed to confirming existing cases). Commence runs in collaboration with QUB. Commence write-up of code (ideally for CPC 50th anniversary special edition). Any final work on theory paper as required by journal. MP to concentrate on He, Li and initial performance/viability tests of noble gases: large-scale work to continue through 2018-2019. SL to provide SESC support for QUB codes as requested. To be carried out when possible by SL's replacement. The initial Flagship support has prioritized UKRmol+ over RMT.	Q3 2017 – Q1 2017

QUANTICS	Quantics parallel load-balancing assessment for Hamiltonian build, followed by (initial) optimization as required (SL, as decided in Q2). Review of work and program for end Q4-Q1 decided. Progressing as planned. To be continued when possible by SL's replacement.	Q3 2017 (into Q4 2017)
TNT	SEG (SL) to commence active support for TNT/CCE as decided in earlier review meeting. Ongoing - Waiting for planning meeting. See above for details (Python work by AK after ML's paternal leave) Note: an internal competition has secured the services of STFC Graduate Tom Dack to provide 3 months' SEG CCPQ work over Q2-Q3 2018. Q1 2018: AK is now working with ML on the Python interface as planned: ongoing	Q3 2017- Q4 2017 Q1 2018 into 2018-19
SBS support	SL to work (separately) with TNT and UKRMol+ (in conjunction with Flagship or as core support) on Build Service integration. Ongoing. Work due to start on UKRmol+ postponed while waiting for input from JDG (and now until CJ reorganizes the group after SL's departure).	Q3 2017- Q1 2018
Novel Technology/ PFARM	Continued novel technology software support as deemed relevant/important (details to be added/reported). AGS, MP maintaining the code. MP was asked to prioritize RMAT_REACT (see above). Note: in Q1 a new application was made for PRACE time to further optimise PFARM for GPUs: this work (by AGS on additional PRACE time) is planned for 2018-19 and will feed back to CCPQ.	Q3 2017 (into Q1 2018) Q1 2018 into 2018-19
Antimatter	Continued advice/support for MML and student (MP) as decided in Q2 meeting (details to be added) Face to face meeting postponed (see above). MML and student should be available in Q2 2018. MP has been working with EAGA on details of integrals for antihydrogen work. A short paper has been written for submission in Q2 2018.	Q3 2017 (into Q4 2017) Q1 2018 into 2018-19
General	General website and other support, as above. Review of objectives. A selection of projects for 2018- 2019 agreed, final plans to be prioritized from them (Q1-Q2 2018). The full CCPQ Steering Panel meeting will be at the start of Q2 2018.	Q3 2017 (into Q4 2017)
Atomic R-matrix	MP to commence work supporting either flagship or relativistic QUB projects as decided. Possible follow-up work with C Ballance (QUB) on PFARM/PSTGF code comparisons (as part of relativistic project support) See above (d-c work prioritized): PFARM/PSTGF comparisons have been built into the HEC proposal as separate support (but may be brought back to CCPQ support if required).	Q4 2017 – Q1 2017
QUANTICS and TNT	Continued support for Quantics and TNT as decided in Q3 review (SL). o be confirmed once SL's replacement is decided by CJ. (see above for details)	Q4 2017-Q1 2018
CCE/TNT	DJ to support (via web bookings) the planned CCPQ Floquet theory workshop as required.	Q4 2017 or Q1 2018

	As of November, support has not yet been requested.	
Flagship (Atomic R-matrix and UKRMol+, SBS)	AGS/MP optimization work for RMT/UKRMol+ as decided in Q3 project meeting (above). SEG ongoing 'Build Service' support as decided (see above). Details to be added. MP: d-c work and RMAT_REACT work. AGS: UKRMol+ memory optimization TR/paper and symmetry/diagonalizer work. SEG: Python and other work as staff are available. See highlighted additions to the above text for details.	Q4 2017 – Q1 2018
General	Implementation of agreed longer term objectives from Q2-Q3 2017 Ongoing: See highlighted additions to the above text and 2018-2019 plans for details. Also: MP: preparation for CCPQ Steering Panel and UK-AMOR initial management meeting in early Q2 (including agreement on provision of 0.2FTE CoSeC support for UK-AMOR). Transfer of CCPQ mailing list(s) to new Listserv server (complete). AK: full upgrade/modernisation to TNT Virtual Machine image distribution plus minor bugfixes (complete).	Q4 2017-Q1 2018

Staffing	**Effort**
Martin Plummer	1.00 FTE
SEG (mainly Steven Lamerton)	0.45 FTE
Andrew Sunderland	0.50 FTE
Total	**1.95 FTE**

CCPQ – Summary Report (1 April 2017 – 31 March 2018)

The SLA/CoSeC support provided solid progress with respect to planned objectives and milestones. One highlight is the completion of a joint computational project with PRACE-funded development work, supervising the successful production of GPU and Xeon Phi 'accelerator' versions of the PFARM R-matrix collision code for general use and to be part of the developing PRACE Unified European Accelerator Benchmark Suite (part of the established Application Benchmark Suite, to enable benchmarking of new architectures and representing a wide range of scientific fields). This complements previous Xeon Phi work on PFARM performed in collaboration with ICHEC. PFARM can be used with CCPQ's ab initio electron atom collision suites and the UKRMol(+) electron (positron) molecule collision suites to produce energy-dependent quantum scattering parameters and matrices. A new objective agreed over the summer was to support ultracold molecular chemistry work at UCL (J Tennyson) by adapting PFARM for heavy particle collisions. Proof of concept calculations have been completed with relatively simple interaction potentials and further work is planned. In addition, CoSeC support assisted with a new HEC proposal (UK-AMOR, PI J Tennyson) to provide the various CCPQ R-matrix communities (ab initio non-relativistic and relativistic electron atom/ion, electron molecule, laser atom/molecule interactions and collisions, plus the new planned ultracold chemistry R-matrix approach) with ARCHER time and scope for sustained HPC-level calculations and additional development support.

Also, memory optimization of the UKRMol(+) suite has continued with results to be presented at the CCPQ Flagship Project meeting at Queen's University at the end of October. Similarly, progress has continued with the new atomic R-matrix double continuum theory and coding, again (to be) presented at the October meeting. The SESC group have agreed a new support programme for the QUANTICS package (G Worth), have improved its continuous integration (CI) environment and begun an optimization project. They have also met with the new Tensor Network Theory PDRA (M Lubasch, Oxford) and agreed to expand previous work on a PYTHON interface script for running the package

(eventually to replace existing MATLAB coding). The project office provided online administration for the Windsor 2017 meeting (TNT and strongly correlated systems).

UKRMol+ Memory optimization work was presented at the Flagship Project meeting, and then further expanded with substantial savings and a Technical Report in progress. The double continuum theory paper was presented at the Flagship meeting and the coding and serious testing is underway as planned. The CCPQ HEC, UK-AMOR, was approved and commences in Q2 2018: preliminary work in advance of official support has taken place with further expansion of PFARM to cope with various general atom-atom potentials The TNT Python work is now underway. A new application for PRACE funding was made, and an internal competition has resulted in securing the services of an STFC Graduate Worker for part of 2018-19 for SEG work (and for training the graduate).

CCPQ – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

Core support for CCPQ can be divided into three main types: detailed scientific and computational collaborative research and code development/optimization, more general best practice software engineering and 'continuous integration' support, and general administration including the CCPQ website. The first type is concentrated in the electron collisions, multiphoton interactions and antimatter areas. This will continue in 2018-2019 complementing the work of the CCPQ Flagship proposal in the 'R-matrix' collisions/multiphoton areas, actively underway to develop and unite the 'RMT' (atomic electrons responding to and ionizing in laser pulses) and 'UKRMol+' (electron/positron-molecule low-energy collisions, excitation and resonance formation) code packages. The R-matrix method effectively solves the time-independent and the time-dependent Schrödinger equation directly for many-electron systems, making use of separate appropriate ab initio treatments for different regions of configuration space, namely the 'inner' region containing the 'target' atom or molecule, and 'outer' regions away from the target containing 1 or, recently, 2 electrons (or positrons). Martin Plummer will continue to have particular responsibility for the latter 'double-continuum' general atom inner region coding, validation/verification, performance and testing for a range of application systems. Andrew Sunderland will undertake various memory and performance optimization projects for the UKRMol+ package. The general coding support will also complement work to be done as part of the new R-matrix HEC. This includes further work on the new R-matrix package for ultracold heavy particle collisions and resonances ('RMAT_REACT'). With the Steering Panel's approval, appropriate CoSeC support will be given following requests from other members of CCPQ's Working Group user community.

Overall, support will be provided by MP, Andrew Sunderland and the Software Engineering Group. Alan Kyffin of SEG is providing support, particularly for the Oxford/Bath Tensor Network Theory (TNT) group. An STFC Graduate, Tom Dack will provide additional support in Q2-Q3 2018. The 'SESC Build Service', previously SL's responsibility, will have new 'ownership' in SEG/SESC and support for CCPQ packages will be maintained. Continuation of optimization work started by SL for the Quantics package for reactive molecular quantum dynamics will be agreed by the start of 2018-2019 (once the best person to do this has been assigned). Damian Jones will continue to support/provide workshop administration as part of central support.

The CCPQ Steering panel will meet in January or February 2018, in fact in early April 2018, and detailed plans (and timescales) will be decided. CCPQ is very pleased that the new UK-AMOR HEC for R-matrix work was approved and limited additional (0.2FTE) CoSeC support added: this will be carried out by AGS with MP's assistance (MP funded from CCPQ support). The {following} table has more detail on which activities are currently agreed as worthwhile/needed for the year.

Staffing	**Effort**
Martin Plummer	1.00 FTE

SEG (mainly Steven Lamerton)	0.45 FTE
Andrew Sunderland	~~0.50~~ 0.55 FTE
Total	~~**1.95**~~ **2.00 FTE**

CCPQ – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

In 2019-20 CoSeC support will continue for the main CCPQ code packages. Direct coding support (and associated scientific collaboration) will be given to the various atomic and molecular R-matrix codes: RMT, UKRMol+ and the 'in-house' PRMAT (PFARM) packages, plus CCPQ support will be combined with additional HEC CoSeC funding to support further development of the Rmat_React ultracold chemistry resonant collisions package. The atomic double-continuum code should in this year be fully evaluated and passed on to users (with support) in the UK-AMOR HEC consortium. The support will help to maintain these packages as internationally leading scientific codes in their areas, and with the assistance of UK-AMOR, extend the codes' impact. SEG's involvement will continue to provide general support for TNT and the Quantics package as required by CCPQ, and appropriate CoSeC support will also be given to other members of the diverse CCPQ community with Steering Panel approval. The types of specific support will follow on from the 2018-2019 work following review in Q4 2018. We will support funding applications for and related to CCPQ as they arise, including the CCPQ renewal call when it is announced, and maintain and promote the website and mailing lists. CoSeC's general support (currently Damian Jones) will provide expertise in setting up registration and payment for workshops. We will ensure that the support provided includes interactions with various university PhD students and PDRAs to provide effective (on the job) training.

CCP-Plasma – HEC-Plasma Physics

CCP-Plasma includes researchers from UK universities, the Culham Centre for Fusion Energy (CCFE), the Rutherford Appleton Laboratory (RAL) and AWE. The study of plasma physics covers a huge range of scales and applications. It is core to the development of laboratory experiments such as fusion power, new light sources and the next generation of particle accelerators. On the largest scales it is fundamental to our understanding of astrophysics.

CCP-Plasma was established in 2007 with the aim of pooling the collective expertise across these disparate subjects and developing core plasma physics simulation codes, and training packages, for UK science. CCP-Plasma supports three core codes EPOCH, BOUT++ and GS2. We also have one Flagship project for the development of a radiation-hydrodynamics ALE code for laser plasmas (Odin). 1FTE of CoSeC core support is split evenly between the codes GS2 and BOUT++, which both focus on modelling plasma in magnetic confinement fusion devices. This CoSeC support is funded 20% from the HEC-Plasma Consortium until 28/5/2023.

The Plasma High-end Computing (HEC) Consortium is an EPSRC funded collaboration of UK plasma physics researchers. The Plasma HEC supports research in the simulation of plasmas, including those plasmas of relevance to magnetic confinement fusion, laser-plasma interactions, and laser fusion energy. The software development includes a commitment to optimizing key codes, with input from EPCC, RAL and Warwick Computer Science, and developing new physics packages as required to maintain the UK's role in laser-plasma physics and all approaches to fusion for energy. The consortium supports meetings and software development. It also manages a block allocation of national super-computer time to be used for plasma physics research.

CCP Plasma/HEC Plasma – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Simulations of the plasma in Magnetic Confinement Fusion (MCF) devices are very expensive due to high dimensionality and multiple scales in both space and time.

Optimizing performance and scalability of plasma codes is vital for efficient use of resources, and for helping to open up the possibility of routine state-of-the-art simulations of physical regimes which are presently inaccessible. The tasks to be delivered by Core Support from STFC focus on maximizing the scalability of the MCF plasma codes GS2 and BOUT++. Both these codes are widely used, and account for a large fraction of the computing time used by HEC Plasma. This optimization work is required urgently so as to maximize the scientific exploitation of these codes for the study of plasma turbulence and instabilities using state-of-the-art HPC systems.

CCPPlasma	Milestone	Target Date
	GS2: Design and implement operator splitting in the time advance algorithm, so that collisions are evolved separately from other terms. Demonstrate the validity of the algorithm and associated improvements to GS2's performance. Complete	Q2 2017
	BOUT++: Optimize the DataIterator object in BOUT++. Parallelize with OpenMP and ensure that it is vectorized by compilers. Complete	Q3 2017
	BOUT++: Profile the performance of BOUT++ v4.0.0 on Archer's conventional nodes and Knights Landing development platform. Compare performance to previous study with BOUT++ v3.0.0. Complete	Q4 2017
	GS2: Develop streamlined version of GS2 with improved layouts/decompositions optimised for scalability and performance: e.g. by implementing the calculation of linear terms in the "gf" memory layout, and parallelizing using shared memory. Demonstrate the achieved improvements to GS2's scalability. Complete – implemented as "split domains".	Q1 2018

Staffing	Effort
Joseph Parker	1.00 FTE
Total	**1.00 FTE**

CCP Plasma/HEC Plasma – Summary Report (1 April 2017 – 31 March 2018)

The project is proceeding as planned with 1FTE from Joseph Parker divided between the codes GS2 and BOUT++.

Minimizing plasma turbulence in tokomaks (nuclear fusion devices) is vital for achieving fusion, but simulations of fusion plasmas are computationally very expensive. GS2 is a plasma turbulence code which has been developed since the 1990's and is already highly optimized; however further optimizations are required for simulations to include all physical effects and to resolve necessary space or time scales. Collisions are vital for the fidelity of turbulence simulations, but introduce a large computational overhead, due to additional calculations and memory redistributions. Collision terms must be calculated twice per timestep (during both the predictor and corrector parts of the time advance), as well as once per grid point during the code initialization. In this reporting period, we have implemented operator splitting so that collisions are evolved separately from the predictor/corrector algorithm used for other terms. Consequently collision terms are now computed once per timestep, rather than twice, and not computed at all during initialization. Depending on core count, this yields a speed up of a factor 1.6 to 4.4 for the initialization, and from 1.1 to 1.6 for the time advance. These significant savings will allow users more routine access to realistic collisional simulations.

We have also implementated "split domains", a more flexible approach to GS2's data layout. The default parallelization scheme splits a single index which represents five physical dimensions uniformly among

available processors. This means that in memory redistributions, these five dimensions are usually not contiguous, and communication patterns can be very inefficient. The split domain option makes this parallelization aware of the underlying five dimensions. The user specifies the number of processors that each dimension should be split over, and data is now held so boundaries in the five dimensions correspond to processor boundaries. This leads to much more efficient communication patterns in memory redistributions, and test problems show a speed-up of a factor 2.25.

Achieving fusion also requires an understanding of plasma behaviour at the tokomak edge, for which BOUT++ is a widely-used code. Since the release of BOUT++ v4.0.0 in February 2017, all loops are performed using the "DataIterator" object, which yields improved performance, syntax and adherance to C++ standards. Initially the DataIterator loops were not optimized. In this reporting period, we parallelized the DataIterator loops with OpenMP (which accounts for one of the three dimensions available for parallelization) and also ensured that the loop would be vectorized by compilers. In addition, we improved the loop performance in serial code by modifying the DataIterator to use a single compound index to access the underlying data, rather than using three-dimensional indices. Now basic looping operators scale ideally to node size on Archer. Furthermore, the optimized looping method is between 1.5 and 5 times faster, depending on the compiler and thread/core counts. These improvements materially contribute to the goal of using BOUT++ for simulations of turbulence in the tokomak edge.

CCP Plasma/HEC Plasma – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

Simulations of the plasma in Magnetic Confinement Fusion (MCF) devices are very expensive due to high dimensionality and multiple scales in both space and time. Optimizing performance and scalability of plasma codes is vital for efficient use of resources, and for helping to open up the possibility of routine state-of-the-art simulations of physical regimes which are presently inaccessible. The tasks to be delivered by Core Support from STFC focus on maximizing the scalability of the MCF plasma codes GS2 and BOUT++. Both these codes are widely used, and account for a large fraction of the computing time used by HEC Plasma. This optimization work is required urgently so as to maximize the scientific exploitation of these codes for the study of plasma turbulence and instabilities using state of the art HPC systems.

GS2 uses different code modules to calculate different physical effects. Historically, these modules have been optimized separately, and each typically uses its own memory layout. Profiling shows that the cost of redistributing data between these different layouts is the main limit to performance and scalability, despite recent work minimizing the number of redistributions. In the first GS2 milestone, we will improve our "split domains" data layout to make it node-aware (as well as processor-aware), and to allow more flexibility in the choice of splits. This layout uses contiguous blocks of data, rather than the uniform blocks currently used. This should significantly simplify communication patterns, by replacing all-to-all communications with communications among groups of processors.

In the second GS2 milestone, we will assess the impact of the new data layout on GS2 performance. We anticipate that performance will be improved, but that the scaling bottleneck in the field solve will remain. This will be due to the communication of arrays (like the electromagnetic fields) which do not have the data layout of the distribution function and which therefore will not have benefited from the above optimizations. We will use shared memory to alleviate this bottleneck, and to help assess whether it will it be necessary to distribute the fields data across processors.

BOUT++ Since the release of BOUT++ v4.0 in February 2017, all loops in BOUT++ are performed using the "DataIterator" object. In recent work, we vectorized and OpenMP-parallelized the DataIterator, yielding a significant performance improvement and ideal scaling of important BOUT++ functions. In

the first BOUT++ milestone, we will extend this optimization work to higher level functions, particularly focussing on optimizing BOUT++'s flagship physics modules, Hermes, Storm and GEMGF. This will ensure code improvements are passed on to users.

The second milestone will focus on BOUT++'s multigrid algorithm for inverting elliptic differential operators. As part of a EUROfusion grant to STFC/CCFE, an algebraic multigrid solver will be implemented by the High Level Support Team at IPP Garching during Q1-Q3 of 2018, to allow BOUT++ to invert a larger class of elliptic operators. We will collaborate with the HLST to ensure the mutligrid solver is implemented and available for users. We will also couple this solver to BOUT++'s implicit time-stepping routines to allow it to be used in preconditioning the time advance. We will develop a preconditioner to allow larger timesteps in turbulence simulations, which are currently strongly limited by fast electron dynamics, even when using implicit timestepping methods.

Staffing	**Effort**
Joseph Parker	1.00 FTE
Total	**1.00 FTE**

CCPPlasma/HEC Plasma – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

GS2 solves the gyrokinetic equations, which describe plasma turbulence on relatively short timescales. To model turbulence in tokomaks on timescales comparable with the plasma confinement time, GS2 is coupled to the transport solver Trinity. After our optimization work on GS2, it is likely that GS2 will no longer be the performance bottleneck in GS2/Trinity turbulence simulations. Therefore in 2019-20, we plan to focus on optimizating the coupling between GS2 and Trinity, and on improving the convergence of Trinity's iterative method.

By 2019, BOUT++ users – particularly those at CCFE with whom we work closely – will be focussing on more realistic simulations of turbulence in the tokomak edge. These simulations will require new functionality in BOUT++, such as including kinetic corrections and non-local effects, and coupling to models to neutrals and plasma impurities. We will implement the new features that are necessary to support these simulations, and ensure that these do not have a negative effect on code performance and scalability.

CCPi – Tomographic Imaging

The CCPi was established in 2012 to support the emerging UK tomography community with a toolbox of algorithms to increase the quality and level of information that can be extracted by computed tomography. In 2015 four major parts were defined to enable modular development of CCPi codes: pre-processing techniques for image calibration and noise reduction, reconstruction techniques to create a 3D volume data set from projections, segmentation and quantification techniques that can extract relevant objective values, and a software framework to enable exploitation within a wide range of existing commercial and open source software environments.

The size of this community has grown over the last five year with many academic groups around the UK taking up tomographic imaging and purchasing new lab based x-ray CT scanners. In 2012 there was an estimated 50,000 CT imaging sources around the world. The size of our community has arisen from ~250 in 2013 to 370 in 2017.

Our focus aims to bring together the UK imaging community in maximising the return on investment in imaging software through developing, maintaining, sustaining and prompting the CCPi core imaging toolbox. Primarily we concentrate on advancing the state-of-the-play of the field through: 1) reducing the barrier to access in multi-modality image analysis algorithms, be the data coming from mid-range

facilities hosted by the universities or from large scale synchrotron or neutron facilities; 2) improving the accessibility and distribution of the codes; and 3) establishing a national multidisciplinary image analysis focal point for the multidisciplinary community comprising of algorithm developers, material scientists, instrument manufacturers, and instrument scientists.

The staffing effort for CCPi core support is as follows: 0.2 FTE for maintaining network, website, running workshops and training course, benchmarking, licensing issues etc; 0.3 FTE enhancing frameworks, 0.3FTE for developing and maintaining the image reconstruction toolbox (including pre- and post-processing), and 0.3FTE for developing and maintaining the 3D image analysis pipeline.

The CCPi core staff actively involves in three major annual imaging events in the country, each having 50+ attendees. These include an X-Ray user group symposium (ToScA) managed by the National History Museum (NHM) and Royal Microscopical Society (RMS), a technical forum supported by RCaH and DLS; and a "dimensional XCT" conference supported by NPL that is leading to formal BSI/ISO standards.

CCPi – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

During the reporting year 2017/18, CCPi plans to deliver two releases of Core Imaging Library (CIL). To the best of our knowledge, the first one will be the first software package worldwide that offers multiscale tomographic image analysis algorithms that covers the entire analysis pipeline, from pre-processing, reconstruction, segmentation, to quantification for cone and parallel beams. We will continue to work closely with our working group, represented by 20+ academics, and our user community (~320 UK based academics and industrialists) to define/refine the algorithms and tools incorporated in CIL. We will work closely with Diamond Light Source, ISIS IMAT and university-based lab imaging centres across the UK to promote best practices through community driven training events. To maximise the impact of our work, we will enhance the quality of data analysis of CT experiments and streamline the analysis process through embedding, deploying, and integrating CIL into three community led image analysis software infrastructure, namely, SAVU (Diamond), ULTRA (STFC facility programme) and at least one university-based lab image analysis workflow.

We will support the CCPi flagship work into multi-channel CT analysis, focusing on enhancing its portability, robustness, distribution, and ease of use when it comes to real world big experiment data.
In the training and presentations front, CCPi will organise three events, including "Tomography for Scientific Advancement Symposium (ToScA)" – a flagship CCPi sponsored conference co-organised with Royal Microscopical Society, CCPi Imaging Fringe Conference, and joint workshop with NPL on imaging standards. We will also actively explore opportunities to organise joint cross-CCP workshops with other CCPs in the imaging theme.

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives Ongoing. New banner added.	Ongoing
	Organise exec committee and working group meetings, as well as monthly show-and-tell sessions Ongoing. Meetings taking place as planned	Ongoing
	Support current training courses and organise developer workshops. Assist in new proposal writing. Two training courses planned. Also doing 1-1 training with ISIS. Met with GSK and demonstrated VR environment using his data. He was very impressed and is looking at doing a training course.	Ongoing
	Set up and run continuous build and test system in ~~CCPForge~~ GitHub.	Ongoing

	Ongoing. Work is being completed using own server instead of CCPForge.	
	Embed framework: DLS/savu – Working on SCARF integration and Phase 2 considers new beamline users Complete. Latest version of savu (v2.0) is now working on SCARF	Q3 2017
	Embed lab based framework: UoM/ UoS/ UoW Ongoing. Working on plugins for lab based machines. Will move in to 2018/19 plans	Ongoing – case studies due Q3 2017
	Help to organise the main ToScA conference; September 2017 Complete. Took place 7-8 September in Portsmouth. CCPi has a booth and is involved with the paper selection process. Taking VR headsets to demo.	Q3 2017
	Optional: Iterative code for the Nikon XTek X-Ray CT accelerated versions (Link/use tier 1 or tier 2 HPC) The focus of the current year has been in creating and distributing the CIL. Now that we have a product we can aim at embedding it into lab based machine. The new hire based in Manchester should lower the barrier for the adoption of the CCPi code in University based machines. Links with other universities have also been made. Will move into next year's plan.	~~Q3 2017~~ Q4 2018
	Add quantitative code examples from the community: see mid-term targets. No data provided by the community. Not required.	Q4 2017
	Embed framework: ISIS/IMAT– working with ULTRA and Phase 2 opens access up to users Ongoing. Starting working with ISIS to analyse their data with our codes. Now have flagship project to specifically look at improving this. Will move into next year's plan.	~~Q4 2017~~ Q4 2018
	Add pre-processing stages beam hardening correction experiments; now to include publications. Publication under review. Submitted changes after reviewer's comments. Still waiting for result. Will move into next year's plan.	~~Q1 2018~~ Q4 2018
	Optional: Optimise projection algorithms from community requests No demand at the moment. Will be easier to proceed if the desired hire from Manchester joins.	Q1 2018

Staffing	**Effort**
Erica Yang	0.10 FTE
Ron Fowler	0.20 FTE
Sri Nagella (Project Manager)	0.60 FTE
Edoardo Pasca	0.60 FTE
Total	**1.50 FTE**

CCPi – Summary Report (1 April 2017 – 31 March 2018)

In the reporting period, the core support effort (1.42 FTE) was provided by Sri Nagella, Ron Fowler, Edoardo Pasca, and Erica Yang. The effort was spent on the major release of the Core Imaging Library (CIL).

CIL: CIL library is a toolbox of algorithms and tools for tomography image preprocessing, reconstruction, quantification, segmentation, and visualisation. This library is embedded into tomography pipeline projects such as SAVU (developed by DLS). This will enable tomography community to improve their data analysis. The major work undertaken during the reporting period was releasing the first public

version of CIL (version 0.9.x). This is the first time in the UK that aims to address the challenges to improve the take up of iterative reconstruction algorithms and is being done with; simple installation, improved documentation, sample codes, and availability of group specific readers/writers.

- Core team has implemented a simple software installation via an Anaconda channel, so only one single command is required. Documentation is available over readthedocs (http://cil.readthedocs.io/en/latest/) and at least one recipe is provided for each algorithm.
- Core team is working with the instrument scientists (Diamond and ISIS) and users in specific university labs to improve the software and reduce the entry barrier. For each hurdle, case studies are planned with the scientists, and these will be reported in the next report.
- Core and Flagship teams have embarked upon the creation of a new framework to enable a quick implementation of new iterative reconstruction algorithms in Python. The framework allows the simple definition of the optimisation problem, with bespoke norm and/or regularisation terms. Two new reconstruction algorithms, FISTA and FBPD, have been added. This aims to significantly improve the quality of the reconstructed volume in the presence of high levels of noise and to allow multichannel reconstruction.
- Core and Flagship teams have developed a regularisation toolbox with 3 regularisation algorithms developed in C/OpenMP and CUDA, wrapped in Python and Matlab. Regularisation can be used for reconstruction or for image denoising.
- Core and Flagship teams have developed a software for the generation of synthetic phantoms for CT. The software allows the creation of 2D/3D/4D phantoms to be used as benchmark of reconstruction algorithms.
- Core team has worked on improving the performance of the topology based segmentation made available on the first release of the software. Working with the scientists in Research Complex at Harwell and Leeds, we have started on a case study

The CCPi flagship: The CCPi flagship project commenced in April 2107. The flagship project will be addressing the issue of multi-channel CT reconstructions by developing novel techniques. From Q4 of 2017 CCPi core team is working closely with the flagship developers (~2 FTE per annum).

CCPi is now collaborating with the CCPPETMR on developing a common interface for the iterative reconstruction algorithms. The SIRF software and CIL, now share a common Python interface.

CCPi – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

During the reporting year 2018/19, CCPi plans to deliver two releases of Core Imaging Library (CIL). Earlier release of CIL included the first set of algorithms with complete reconstruction pipeline, starting from removing the noise in raw tomography images to reconstructing the projection images to 3D volume, segmenting and quantifying the results. The following release of CIL will improve on the performance of the algorithms and add new algorithms for improving the CT analysis process. We will continue to work closely with our working group, represented by 20+ academics, and our user community (~320 UK based academics and industrialists) to define/refine the algorithms and tools incorporated in CIL. We will work closely with Diamond Light Source, ISIS IMAT and university-based lab imaging centres across the UK to promote best practices through community driven training events. To maximise the impact of our work, we will enhance the quality of data analysis of CT experiments and streamline the analysis process through embedding, deploying, and integrating CIL into three community led image analysis software infrastructure, namely, SAVU (Diamond), DAaS (STFC facility programme) and at least one university-based lab image analysis workflow. For the reporting year, we are planning to work with international collaborators in including Digital Volume Correlation (DVC) as part of CIL. This will improve strain measurements in the CT experimental mechanics, materials science and biomechanics.

Together with University of Manchester we will provide a pipeline to perform laminography on Nikon lab machines, task that is currently not possible. Core team will provide the reconstruction software within

the newly created reconstruction framework, so that a complete pipeline from acquisition to reconstructed laminography volume can be achieved.

We will support the CCPi flagship work into multi-channel CT analysis, focusing on enhancing its portability, robustness, distribution, and ease of use when it comes to real world big experiment data.

In the training and presentations front, CCPi will organise three events, including “Tomography for Scientific Advancement Symposium (ToScA)” – a flagship CCPi sponsored conference co-organised with Royal Microscopical Society, CCPi Imaging Fringe Conference, and joint workshop with NPL on imaging standards. We will also actively explore opportunities to organise joint cross-CCP workshops with other CCPs in the imaging theme

Staffing	**Effort**
~~Erica Yang~~	~~0.10 FTE~~
~~Ron Fowler~~	~~0.20 FTE~~
~~Sri Nagella (Project Manager)~~	~~0.60 FTE~~
Edoardo Pasca	~~0.60~~ 0.56 FTE
New Hire	1.00 FTE
Total	~~**1.50**~~ **1.56 FTE**

CCPi – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

The Core team will focus on releasing the CIL with a 6 monthly stable release plan. The main additions to the CIL are expected to be with the Digital Volume Correlation (Brian Bay, USA) and new machine learning for tomography (e.g. identification of zingers, selection of region of interest).

The Core team will continue to give support to the Flagship team in the image reconstruction, and support the community (Diamond, ISIS/IMAT) with their software.
Distribution of the CIL software will be on conda channel and virtual machines running on the SCD Cloud based on DAaS will be provided.

The core team will still provide support to the community via the website, mailing list and by organising conference and meetings.

CCP-PET/MR - Positron Emission Tomography (PET) and Magnetic Resonance (MR) Imaging

For medical imaging, the UK is a globally leading country. It has the highest number of Positron Emission Tomography and Magnetic Resonance (PET-MR) medical imaging machines per capita in the world, evenly spread throughout the country. The CCP PET-MR project established in 2015 aims at bringing together the best of the UK’s PET-MR imaging expertise to capitalise on the investment in this area. New research shows that the use of MRI intermediate results can improve PET imaging quality and vice versa, and latest scanners can acquire MR and PET data simultaneously. Our CCP is dedicated to exploiting exciting new capabilities that the synergy of MR and PET imaging can deliver. The main deliverable of the project will be an open source PET-MR reconstruction software framework we named SIRF (Synergistic Image Reconstruction Framework). SIRF will be simple enough in use for educational and research purposes, thus reducing the “barrier for entry” for new contributors to PET-MR imaging research and development, and at the same time powerful enough to process real scanner data.

STFC CoSeC support for this CCP currently focusses on developing the SIRF code base that provides an easy-to-use script-language (Python and Matlab) environment built around existing open source reconstruction software. This includes maintaining network, website, running workshops and training

courses, on top of the software engineering effort that contributes to SIRF development, testing, deployment and documentation.

CCP-PetMR – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

In 2017/18 we plan to continue our software development effort, publishing SIRF Release 1.0 in the last quarter of 2017 and Release 2.0 in the second quarter of 2018. Release 1.0 will include SIRF Developer's Guide, in addition to User's guide, and inline documentation in C++ sources, facilitating contributions to our code development from the wider CCP PET-MR community. Windows installation issues will be addressed, possibly employing pre-installed libraries, in order to reach for a sizeable Windows' users' audience. Release 1.0 will take into account scattering effects in PET, thus improving the accuracy of the reconstruction. Release 2.0 will be the first one to deliver synergistic PET-MR reconstruction by bringing PET and MR image objects under one roof and using MR-reconstructed images as anatomical priors for PET reconstruction.

We will continue to engage with the CCP PET-MR community by maintaining our website and mailing lists, organizing meetings, developers' days and other events. We will continue to organize and support training courses and developers' workshops and assist in new proposal writing. Our embedding within Institute of Nuclear Medicine at UCL Hospital for two days a week, proved to be extremely beneficial to our software development effort, will continue in 2017/18, and similar arrangements with KCL will be sought.

CCPPET-MR	Milestone	Target Date
	Manage CCPPETMR website, mailing lists and data archives for both simulated and acquired data. Ongoing	Ongoing
	Organise exec committee, working group meetings, developers days and other event sessions Ongoing	Ongoing
	Support current training courses and organise developer workshops Ongoing	Ongoing
	Assist in new proposal writing. Ongoing	Ongoing
	Visit sites in the network to gain experience with a few selected packages for image reconstruction and to get others started with SIRF Ongoing	Ongoing – embedding two days a week
	Set up and run continuous build and test system in CCPForge Abandoned	Abandoned due to the closure of CCPForge
	SIRF Release 0.9. Complete – released June 2018	Q2 2018
	Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide. Ongoing	Ongoing
	More real data functionality (import of raw data, PET randoms, norm and scatter), excluding GE raw MR data. Ongoing	Ongoing
	Optional: Profiling (and possibly speed-up) of PET reconstruction. Ongoing	Ongoing

	Write SIRF installation script for Windows, possibly using pre-compiled libraries. In progress. Deadline shifted because of the higher priority of real data processing capabilities. Will move into next year's plans.	~~Q3 2017~~ Q2 2018
	SIRF Release 1.0. Complete – April 2018	Q4 2017
	Implement image data transformations between PET and MR and between different voxel grids and encapsulate image data into common SIRF image object. Ongoing. Deadline slipped because of the delay with Release 1.0. Will move into next year's plans.	~~Q1 2018~~ Q2 2018
	Implement PET reconstruction with MR anatomical priors. Deadline slipped because of the delay with Release 1.0	~~Q1 2018~~ Q2 2018
	Implement iterative MR reconstruction with Gadgetron. Deadline slipped because of the delay with Release 1.0	~~Q2 2018~~ Q3 2018
	SIRF Release 2.0 Deadline slipped because of the delay with Release 1.0	~~Q2 2018~~ Q4 2018

Staffing	**Effort**
Erica Yang	0.10 FTE
Evgueni Ovtchinnikov (Project Manager)	1.00 FTE
Edoardo Pasca	0.40 FTE
Total	**1.50 FTE**

CCP-PetMR – Summary Report (1 April 2017 – 31 March 2018)

Our work during the reported period progressed according to the job plan: software development and engineering efforts, adding content to our website www.ccppetmr.ac.uk, maintaining mailing lists (we now have 88 members on the CCP-PETMR announcement list, 18 on the developers and 60 on the users lists), organising working group and executive meetings, organising a series of well-attended Developers Days' to present and discuss progress in our software framework development.

The first two public releases of our open source software suite SIRF took place in June (Release 0.9.0) and September (Release 0.9.2) 2017, and SIRF Release 1.0.0 took place on 3 April 2018. These releases are based on the PET reconstruction package STIR (Software for Tomographic Image Reconstruction) and the MR reconstruction package Gadgetron, and Release 1.0.0 provides initial support for Siemens mMR PET data reconstruction. The SIRF distribution includes source code, installation instructions and scripts, test scripts, demo scripts and several layers of documentation. An Oracle Virtual Machine (VM) is also provided that has all the necessary software (except, for licensing reasons, Matlab) pre-installed for a quick start in any operating system that supports VMs. All this software is available for free download on our public website www.ccppetmr.ac.uk and via github.com/CCPPETMR.

We have obtained official agreement from GE Healthcare to provide open source software for reconstructing of their PET data, directly from the raw data from the scanner, i.e. disclosing the previously confidential file format. We have received considerably help and code from GE. This capability is now being incorporated into STIR at UCL and Leeds (due to the nature of the agreement). In addition, postdocs and students at Hull, UCL and Leeds have added Time-Of-Flight capabilities to STIR. These additions are under final stages of development and testing by participants in our community. This code will also be applicable to GE PET/CT systems, increasing the impact of our work considerably.

Researchers at the PTB (Germany) have acquired a test-suite of MR data to test capabilities for Siemens MR scanners with good results. Some issues were uncovered related to repeated sequences and orientations. These are now being addressed.

The development of SIRF opens up significant opportunity for the user community to adopt or test the codes in a real PET-MR system. For the first time ever the community will have access to a software system that facilitates end-to-end PET-MR imaging method testing, from pre-processing to reconstruction to post-processing, all under one software framework. We expect that this new development will significantly ease the efforts and time required to test and validate PET-MR methods and algorithms.

CCP-PetMR –2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

In 2018/19 we plan to continue our software development effort, publishing SIRF Release 2.0 in the last quarter of 2018. Release 2.0 will be the first one to deliver synergistic PET-MR reconstruction by bringing PET and MR image objects under one roof and using MR-reconstructed images as anatomical priors for PET reconstruction and vice versa. It will be able to perform PET reconstruction with MR anatomical priors and provide full support for measured data (Siemens, GE non-Time-Of-Flight, MR only if ISMRMRD converter available) and PET Time-Of-Flight support (no scatter). Our subsequent effort will be directed at motion estimation and motion-guided reconstruction and MR reconstruction with PET prior. We will continue our engagement with the CCP PET-MR community by maintaining our website and mailing lists, organizing meetings, developers' days and other events. We will continue to organize and support training courses and developers' workshops and assist in new proposal writing. Our embedding within Institute of Nuclear Medicine at UCL Hospital for up to two days a week will continue in 2018/19, and similar arrangements with KCL will be sought.

Staffing	**Effort**
~~Erica Yang~~	~~0.10 FTE~~
Evgueni Ovtchinnikov	1.00 FTE
Edoardo Pasca	0.40 FTE
Total	~~**1.50**~~ **1.40 FTE**

CCPi – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

In 2019/20 we plan to continue our software development effort aiming at joint motion estimation and joint PET-MR reconstruction using MATLAB or Python tools/toolboxes, list mode reconstruction without conversion to sinograms, time-of-flight reconstruction and the employment of some generic optimization algorithms. We plan to have most of these features in SIRF Release 3.0, to be published in the second quarter of 2019. We will look into SIRF code optimization issues, possibly involving GPU implementation. We will investigate the possible use of non-cuboid voxelization (non-Cartesian grids, wavelets, blobs etc.). We may also consider the integration of other reconstruction packages into SIRF. We will continue our engagement with the CCP PET-MR community by maintaining our website and mailing lists, organizing meetings, developers' days and other events. We will continue to organize and support training courses and developers' workshops and assist in new proposal writing. Our embedding within Institute of Nuclear Medicine at UCL Hospital for up to two days a week will continue, and similar arrangements with KCL will be sought. Last but not least, we will seek the continuation of EPSRC support and look for other sources of funding for our PETMR research and development efforts beyond 2020.

CCPBioSim - Biomolecular Simulation at the Life Sciences Interface

CCPBioSim is the Collaborative Computational Project in biomolecular simulation at the life sciences interface, bringing together chemists, physicists and chemical engineers as well as researchers from all branches of "molecule-oriented" biochemistry and biology. Simulations help to analyse how enzymes catalyse biochemical reactions, and how proteins adopt their functional structures e.g. within cell membranes. They contribute to the design of drugs and catalysts, and in understanding the molecular basis of disease. Our aim is to involve experimentalists and computational specialists in this work, sharing the belief that the best science can be done when theory and experiment are closely integrated. CCPBioSim engages with early career researchers and non-experts through the provision of tutorials and workshops enabling them to become proficient and productive users of biomolecular simulation techniques. We are also actively engaged in developing new advanced methods, which in future will be used by our community to deliver new and exciting science.

CCPBioSim is supported by 1.2 FTE of SLA core effort with 0.2 FTE to support coordination of SLA effort, networking activities including organization of conferences and training, and 1.0 FTE to support software development of tools of benefit to the community. For further information please see www.ccpbiosim.ac.uk.

CCPBioSim – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

For networking activities, 0.2 FTE of SLA core support will be used to support collaboration tools, and organization of conferences and training. The remaining 1.0 FTE will be used to support software development on tools of benefit to the community.

Networking activities:

- Organisation of the 3rd CCPBioSim/CCP5 multiscale modelling conference with support from academic representatives of the two CCPs and the SLA project office. The conference is expected to be held in April 2018 in Manchester.
- Organise a CCPBioSim ChemShell QM/MM training workshop in Daresbury (9 May 2017).
- Help organize the joint CCP5/CCPBioSim “Simulations for the Experimentalist and Industrialist” training workshop series.
- Assist with the organization of other workshops and events as required. This usually involves handling the registrations and any associated fees by the SLA project office, though additional help can be given to the local organisers as needed.
- Manage the CCPBioSim email list ccpbiosim@jiscmail.ac.uk
- Support use of the code repository CCPForge, for dissemination and curation of software outputs, simulation movies, interactive demos, scripts and protocols. Where appropriate, access would be via the CCPBioSim website.

Software development:

- Continue development of FESetup:
- Support for arbitrary mutations e.g. protein side-chains (“partial molecules”)
- LOMAP2 integration (see below)
- Longbow integration to load-off expensive calculations
- ProtoMS support
- Clean-up of hard-coded filenames in perturbed topology writer to increase usability for less experienced users
- smaller changes like: arbitrary box shapes, increase robustness e.g. check quality of ligand force field, better equilibration protocols e.g. single keyword, pre-equilibration of perturbed setup

- Technical improvements like switch-over to Python 3, refactoring to accommodate new developments, conda support, etc.
- Co-development of LOMAP2 (David Mobley, UC Irvine, US). This will be used to compute the similarities and minimum path for large set of ligands and integrated into FESetup. LOMAP2 will also include support for binding modes (with some ideas developed in FESetup) and chirality.
- Discuss with Michael Shirts (University of Colorado, Boulder) and others the development of a general topology conversion program e.g. on the basis of Intermol and ParmEd.

CCPBioSim	Milestone	Target Date
	Hold ChemShell training workshop for biomolecular QM/MM modelling Complete, held on 9th May at Daresbury.	Q2 2017
	Complete free energy reproducibility study Complete	Q3 2017
	Lead organisation of the 3rd CCPBioSim/CCP5 Multiscale Modelling Conference Organisation proceeding on track for meeting on 21-23 May 2018	Ongoing (to be held Q2 2018)
	Longbow integration Postponed due to CCPBioSim staff member leaving during this reporting period. FESetup code to be fully reviewed before further development work is undertaken.	~~Q2 2017~~ Postponed pending code review
	ProtoMS support Postponed due to CCPBioSim staff member leaving during this reporting period. FESetup code to be fully reviewed before further development work is undertaken.	~~Q2 2017~~ Postponed pending code review
	LOMAP2 integration Postponed due to CCPBioSim staff member leaving during this reporting period. FESetup code to be fully reviewed before further development work is undertaken.	~~Q3 2017~~ Postponed pending code review
	General clean-up and usability improvements Complete; released FESetup version 1.2.1 with numerous bug fixes, general clean up and usability improvements	Q4 2017
	Review MD and QM/MM tutorials on ccpbiosim.ac.uk Complete	Q1 2018
	Support for side chain mutations (FESetup 2.0) Postponed due to CCPBioSim staff member leaving during this reporting period. FESetup code to be fully reviewed before further development work is undertaken.	~~Q1 2018~~ Postponed pending code review
	FESetup code review Complete	Q1 2018

Staffing	Effort
Hannes Loeffler	1.00 FTE
Thomas Keal	0.20 FTE
Total	**1.20 FTE**

CCP-BioSim – Summary Report (1 April 2017 – 31 March 2018)

Hannes Loeffler's work on FESetup in this period focused on bug fixes, code refactoring and general usability improvements, which have been released as v1.2.1 of the code. Hannes also completed work

on a reproducibility study of relative alchemical free energies in AMBER, GROMACS, CHARMM and SOMD using FESetup.

Hannes left STFC in September to take up a new position in the pharmaceuticals sector. His work on the new FESetup release was prioritised in order to leave the code in the best possible condition for Hannes's successor in the CCPBioSim software development role. Interviews were held at Daresbury on 22/23 November for the position, and Sarah Fegan was appointed, beginning work at the end of January. Since starting Sarah has familiarised herself with the use of FESetup and undertaken a thorough code review in preparation for future developments. She has also attended training courses in other relevant codes developed by CoSeC including ChemShell for multiscale biomolecular QM/MM calculations which will be another focus of future development work. Sarah has also reviewed MD and QM/MM tutorials on the CCPBioSim website both to gain further insight into the wide range of science covered by CCPBioSim and to bring them up to date for the community.

A CCPBioSim training workshop "QM/MM modelling of biomolecular systems with ChemShell" was held on 9 May 2017 at Daresbury Laboratory, combining training lectures on a theme of biomolecular modelling with hands-on practical sessions. Tom Keal led the course with Richard Lonsdale (AstraZeneca) and You Lu (STFC) also contributing talks.

Tom Keal is also leading the organisation of the 3rd CCPBioSim/CCP5 Multiscale Modelling Conference to be held at the University of Manchester on 21-23 May 2018. The event will be held again at the Manchester Conference, and eight invited speakers have confirmed their attendance: Sarah Harris (UK, Leeds), James Kermode (UK, Warwick), Misbah Sarwar (UK, Johnson Matthey), Tomas Kubar (Germany, KIT), Florian Muller-Plathe (Germany, Darmstadt), Ali Karimi (Germany, Continental), Rommie Amaro (US, UCSD), Berend Smit (US, Berkeley). Registration closed on April 9th with 68 registrations received, and a full schedule will be published at the end of April.

CCP-BioSim – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

CCP-BioSim is the Collaborative Computational Project in biomolecular simulation at the life sciences interface. SLA core effort will continue to support CCP-BioSim networking activities and software development. 1.0 FTE will be used to support software development on tools of benefit to the community. The remaining 0.2 FTE of SLA core support will be used to supervise the software development work, support collaboration tools, and organization of conferences and training.

Networking activities:

- Organisation of the 3rd CCPBioSim/CCP5 multiscale modelling conference with support from academic representatives of the two CCPs and the SLA project office. The conference will be held in Manchester on 21-23 May 2018.
- Organise a CCPBioSim ChemShell QM/MM training workshop in St Andrews on 14 June.
- Help organize the joint CCP5/CCPBioSim "Simulations for the Experimentalist and Industrialist" training workshop series.
- Assist with the organization of other workshops and events as required. This usually involves handling the registrations and any associated fees by the SLA project office, though additional help can be given to the local organisers as needed.
- Manage the CCPBioSim email list ccpbiosim@jiscmail.ac.uk
- Support use of the code repositories on CCPForge and github, for dissemination and curation of software outputs, simulation movies, interactive demos, scripts and protocols. Where appropriate, access would be via the CCPBioSim website.

Software development and associated activities:

- The CCPBioSim code FESetup will continue to be maintained and developed further following recruitment of Sarah Fegan as CCPBioSim software developer. Reviewing of the code will be completed including fixing any open technical issues, and a comprehensive benchmark set for relative alchemical binding free energies will be created, to prepare for the integration of FESetup into the BioSimSpace flagship software development project. Work will begin on the development of the metadynamics grand challenge for BioSimSpace.
- The outputs of the first CCPBioSim software flagship project (multiscale modelling of membrane-bound cytochrome P450 enzymes) will be developed further for the benefit of the CCPBioSim community. The protocols and scripts for coarse-grained, atomistic MD and QM/MM simulations originally developed under this project will be refactored for ease of use, curated and made available in a publicly-accessible repository. QM/MM calculations on the system will be benchmarked on ARCHER using the ChemShell QM/MM package as a platform for further development of the models, and will be used to help validate the new open source Py-ChemShell QM/MM software.
- Reviewing of the new CCPBioSim website tutorials section will be completed though validation and refinement of the training materials provided by members of the consortium.

Staffing	**Effort**
~~Hannes Loeffler~~ Sarah Fegan	1.00 FTE
Thomas Keal	0.20 FTE
Total	**1.20 FTE**

CCPBioSim – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

FESetup will continue to be maintained and developed for the benefit of the CCPBioSim community, including the integration of FESetup and the Longbow job submission engine, and support given to the BioSimSpace flagship software development project including development of a BioSimSpace metadynamics node for binding kinetics calculations based on GROMACS/Plumed. The 4th multiscale modelling conference will be planned to be held in 2020 in Manchester. A further CCPBioSim QM/MM training workshop will be held in Daresbury and support given to other training workshops.

MCC – Materials Chemistry Consortium

The Materials Chemistry Consortium exploits high end computing in a broad programme of work modelling and predicting the structures, properties and reactivities of materials. The consortium is a broadly based but coherent grouping comprising 36 university groups, with the emphasis on modelling at the atomic and molecular level but with growing links to models at larger length and time scales. Founded in 1994, the current scientific programme is built around seven related themes: catalysis, energy storage and generation, surface and interfacial phenomena, nano- and defect structures, soft matter, biomaterials, environmental materials. The Consortium has an active programme of code development and optimisation, tapping into the ecosystem of UK based software development initiatives including CoSeC.

CoSeC supports the consortium across the range of techniques used by its members, embracing both force-field methods employing static and dynamical simulation methodologies and electronic structure methods with a strong emphasis in recent years on Density Functional Theory (DFT) techniques employing both periodic boundary conditions and embedded cluster implementations. The four main codes supported by CoSeC are: DL_POLY, DL_FIELD, CHEMSHELL, and CRYSTAL.

MCC – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

CRYSTAL: The work carried out in support to MCC is devoted to the implementation of new functionalities in the CRYSTAL code, to porting the code to super-computers used by MCC members

and to carry out scientific work based on these developments. In previous years we have presented a new implementation of the time-dependent density-functional theory (TD-DFT) method in CRYSTAL, which allows one to study with unprecedented accuracy complex physical phenomena arising from the interaction of radiation with condensed matters, like absorption of light in new material phases, the prediction of UV and visible optical response and the study of the properties of excited states in extended systems, particularly crystalline semiconductors (see e.g. the recent review by Byun and Ullrich in Phys. Rev. B 95, 205136 (2017)). The work planned this year aims to extend substantially the range of applicability of the CRYSTAL TD-DFT method in solids. In particular, we want to consider situations in which excited states retain a delocalised conduction-like character, as opposed to localised excitonic states. For this purpose, we need to re-engineer the algorithms implemented in CRYSTAL for the calculation of two-electron integrals, in particular the exchange integrals, to allow the proper treatment of conduction states. These development will impact the ability to describe reliably the response of solids and other extended samples to wider ranges of radiations (from IR, to visible and UV, to X-rays). This work is being done in collaboration with the main CRYSTAL developer group at the University of Turin (Italy), the University of Oxford and Imperial College London.

We are also involved in several research projects, with a specific focus on the study of homogeneous catalysis (in particular processes for energy production and storage, fuel production and complex isomerisation reactions of relevance in synthetic and industrial chemistry), photo-induced dynamics in new molecular species of relevance in cancer research and in the study of fundamental processes induced by interaction of crystals with ionising and non-ionising radiation.

ChemShell: With the initial release of Python-ChemShell expected during this reporting period, MCC support will be focussed more directly on the Python. 0.1 FTE of MCC support was committed for TWK to supervise the ChemShell developments in the MCC flagship grant proposal, and this effort will start this year. Of the remaining effort, 0.1 FTE will be used to continue support for Tcl-ChemShell on HPC systems used by the MCC community and to maintain Python-ChemShell on the same systems after release. 0.2 FTE will be targeted at new scientific methods in Python-ChemShell, taking the code's capabilities beyond what was achievable with Tcl-ChemShell. In particular, TWK will implement an extension of the "frozen density embedding" scheme for large scale quantum mechanical calculations, where part of the system is treated at an approximate (fixed) level, to allow multiple regions to be frozen and "thawed" in turn, to give greater consistency and accuracy to the result. The final 0.1 FTE of effort will be put towards improving the usability of the DL-FIND geometry optimisation library in ChemShell, particularly focussing on diagnostics to monitor the optimisation of whole chemical reaction paths, which will give MCC researchers greater insight into catalysts and other reactivity of interest.

DL_POLY: With increased supervision effort on the DL_POLY project personal development effort will focus in and target the release and testing of the (i) two temperature thermostat model (TTM) and bring advancements to (ii) multipolar electrostatics (MPE) methodology. Collaborative support and training organisation in collaboration with CCP5 and UKCOMES will continue to be provided.

DL_FIELD: More new features relate to inorganic materials will be introduced such as freeze and tethering of atoms, introduction of three-body potentials, for glassy materials, etc. In addition, further tests will be carried out to ensure the robustness of DL_FIELD capabilities to handle mixed bio-inorganic potentials. From such, some form of automation of setting up mixed parameters will be implemented between the inorganic and organic components.

MCC	Milestone	Target Date
ChemShell / DL_FIND	(Supervision of ChemShell work package in MCC flagship project – subject to funding decision) Project approved, Supervising You Lu who started in August.	Ongoing

	~~Implementation of freeze and thaw frozen density fragment optimisation in Python ChemShell~~ In discussion with community, this was de-prioritised. New target: Complete the porting of the cluster cutting module to python Chemshell. Complete and ready for release in Py-ChemShell 2018.	Q1 2018
	~~Improve usability of nudged elastic band method in DL-FIND through improved initial path guesses, optimisation diagnostics and additional tutorials~~ In discussion with community, this was de-prioritised. New target: integration of DFTB+ code as a fast semi-empirical DFT method. Complete and ready for release in Py-ChemShell 2018.	~~Q3 2017~~ Q1 2018
	Support for ChemShell and GAMESS-UK on ARCHER Released Chemshell3.7 in July, now a module on ARCHER.	Ongoing
DL_POLY / DL_FIELD	Supervision of work, verification and integration of Alin Elena (thermal conductivity), Aidan Chalk (RDF+errors), preparation of DL_POLY for python interfaces RDF+errors done, thermal conductivity is in progress, and python interface is long-term ongoing project	Ongoing
	Collaboration with Graeme Day on real examples of organic crystals MD modelling using multipolar FFs and self-polarisable multipolar FFs. Put on hold, in consultation with community prioritised integrated the two-temperature thermostat work, and this will be released in Q4 2017	Q2 2017
	Two temperature Model integration Complete	Q3 2017
	DL_POLY 25th Anniversary Conference Complete	Q4 2017
	Preparation and lectures of DL_POLY_4 at DL_Software workshops Completed for the last training	Ongoing
	Support for DL_POLY_4 on ARCHER (ITT). Support for DL_FIELD (CY) Ongoing, everything is up to date on ARCHER and any other system MCC members have asked for assistance with	Ongoing
DL_FIELD	Implementation of new inorganic features Complete	Q2 2017
	Reorganisation of inorganic FF libraries Complete	Q3 2017
	Automation of setting up mixed organic/inorganic Postpone to Q4 – 2018, see 2018/19 plans	Q1 2018
CRYSTAL	Merge of UK and Italy version of CRYSTAL17 for release Complete, CRYSTAL17 officially released in September.	Q2 2017
	Paper on multiferroic GaFeO3 – in collaboration with N. Harrison and R. Cernik Stalled. Waiting for experimental collaborators to get back to us.	Q2 2017
	Paper on dynamics of molecules in solution – in collaboration with T. Parker and R. Bisby Draft complete	~~Q2 2017~~ Q4 2017

	Compilation and testing of CRYSTAL17 on Archer and STFC clusters Complete. CRYSTAL17 is available on ARCHER	Q2 2017
	Tests of massively parallel version of CRYSTAL17 on large disordered systems. In collaboration with Dr I Bush (Oxford University) Complete. Testing new DIIS solver of CRYSTAL17. Task has been expanded to test more new implementations.	Q1 2018
	Leonardo to visit Turin University for discussion about current CRYSTAL developments. Barry Searle to visit Turin in May 2018 with Ian Bush to update the Turing group about OpenMP-MPI parallelism work. See 2018/19 plans.	Q4 2018
	Draft of paper on dynamics of catalytic molecules in solution, in collaboration with ISIS. (Dr N Holzmann and LB) Paper accepted in ACS Catalysis (DOI: 10.1021/acscatal.8b00199)	Q2 2017
	Working version of hybrid RPA/coupled-perturbed solver for excited states in CRYSTAL. Examples on molecules and model crystals with pure density functionals and TD kernels. Complete for pure DFT	Q2 2017
	Draft of paper of photo-induced dynamics of anti-cancer drugs, in collaboration with the STFC Central Laser Facility (Dr N Holzmann and LB) Paper accepted (Chem. Phys. Lett. 692, 146-151 (2018)).	Q2 2017
	LB to deliver 4 lectures and 3 half-day tutorials at CCP5 summer school on molecular simulation at Lancaster University. Complete	Q2 2017
	Discussion with ISIS concerning set up of calculations for photo-induced dynamics in solvated Ru-catalysts and potentially plans for joint theoretical-experimental work (Dr Nicole Holzmann and LB) Complete	Q3 2017
	Organise MSSC2017 CRYSTAL summer school and Imperial College London and deliver 5-6 lectures (TBC) and tutorials. Complete – about 33 registered participants	Q3 2017
	Work on massively parallel version of CRYSTAL17 to be extended (potentially) to biological samples. Compile list of potential systems to be considered and set up calculations. Started discussions with people at Diamond (MX group) about which systems to include	Q1 2018

Staffing	**Effort**
Leonardo Bernasconi	1.00 FTE
Barry Searle	0.22 FTE
Ilian Todorov	0.75 FTE
Tom Keal	0.50 FTE
Total	**2.47 FTE**

MCC – Summary Report (1 April 2017 – 31 March 2018)

Computational Physics (CRYSTAL): The software development work in CRYSTAL has been proceeding steadily and according to the plans. The two main branches of development are (1) the extension of CRYSTAL to excited states (TD-DFT, TD-HF and hybrid TD-DFT/HF for periodic systems)

and (2) the implementation of hybrid OpenMP/MPI parallelism in the calculations of the two-electron integrals in the core routines of CRYSTAL. The first class of developments targets one of the priorities identified by MCC communities of CRYSTAL users concerning the accurate and efficient description of electronic excitations (electron-hole pair creation and excitonic effects) in the context of New Materials for Energy Generation. Substantial progress has been made in the last few years to make CRYSTAL a robust code for the ab initio treatment of electronic excitations in solids and amorphous systems, and the current work concerns important extensions of the code to treat wider ranges of excitation energies (optical, UV and X-ray radiation) and to provide a more general and accessible tool for non-expert users. The hybrid OpenMP/MPI parallelism is also an important addition to CRYSTAL, which will make the code more easily portable to modern hardware, in addition to improving the internal structure of the code.

In addition to the CRYSTAL software development work, we have also been involved in a series of UK and international scientific collaborations on projects concerning catalysis, ab initio molecular dynamics and the quantum-mechanical treatment of very large systems, including biomolecules. A substantial effort has been devoted to training (see details in the Workshops and New Opportunities section) and one-to-one interactions with code users. The feedback we have received concerning potential issues that beginners users of CRYSTAL frequently encounter will be relevant for future plans aimed at improving code usability (e.g. choice of basis sets and convergence issues for complex systems). A new version of CRYSTAL (CRYSTAL17) has been officially released in September 2017, it has been ported to Archer and to the STFC SCARF cluster and is now available for registered CRYSTAL users.

Computational Chemistry (DL_POLY, DL_FIELD, and ChemShell/DL-FIND): DL_POLY, DL_FIELD and ChemShell are the most used and actively developed projects at the Computational Chemistry Group at STFC. Support for these codes is provided on ARCHER as well as other HPC platforms of interest to the MCC community.

Chin Yong (0.14 FTE) is focused on promoting inorganic capabilities for organic-inorganic interfaces. He released DL_FIELD version 4.1.1 (April) before the DL_Software training at QMUL. Ilian Todorov (0.61 FTE) supervises the DL_POLY team funded by CCP5 (a new starter January, a new starter March), EPSRC flagship proposal (a new starter November) and IPCC (testing emerging technologies and prototyping acceleration paradigms). Dr. Kostya Tratchenko at QMUL, started using DL_POLY_4 for his master course in Molecular Simulations and Molecular Simulation research by Prof. Nora de Leeuw et al. using DL_POLY made the front cover September Issue of Journal of Molecular Chemistry B..

Dr. Thomas Keal leads the ChemShell project. With his supervising efforts on the MCC eInfrastructure flagship project (started in August) an initial prototype interface to the periodic DFT code CP2K supporting single point calculations is now in place. His teams' work on MCC focussed on completing the port of the cluster cutting module to Py-ChemShell. This critical set of routines for MCC users is now fully functional. A new interface to DFTB+ was also developed for fast semi-empirical DFT calculations. Maintenance and support for the legacy Tcl-ChemShell and GAMESS-UK also continues to be provided, with the latest version of Tcl-ChemShell (v3.7) now available on ARCHER. Support was provided by Tom Keal at 0.5 FTE from April-December 2017, and by Tom Keal at 0.3 FTE and You Lu at 0.2 FTE from January-March 2018 (with You Lu working on the cluster cutting module).

The DL_Software and Hack Day events organised at QMUL April 5-7, 2017 were attended by 20 participants. Dr. Ilian Todorov gave three lectures at the CCP5 Summer School at University of Lancaster, in July 2017. The 10 days' school was attended by 67 participants from all over the world. The school involved not only distinguished academic speakers but also trainers and lecturers from other CoSeC consortia such as HEC-MCC, UKCOMES, UKCP and CCP5. Dr. Chin Yong gave a DL_Software presentation at an ADDoPT technical workshop at Leeds in July. The DL_Software and

Hack Day event at University of Strathclyde, 13-15 September, attracted 15 participants, and a further DL_Software training event was held at Daresbury Laboratory from 19-22 February 2018.

With organisation led by Dr. Ilian Todorov, the organisation of the special meeting to celebrate the DL_POLY projects' 25th anniversary at Chicheley Hall on 3rd November was held. Major stakeholders and power user researchers are confirmed as speakers. The event was sponsored by STFC, CCP5, HEC-MCC, EMCS and Molecular Simulations.

MCC – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

As part of the renewal of the Materials Chemistry Consortium SLA support for MCC has been reduced from 2.5 FTE to 2.0 FTE from November 2018. We have accordingly revised the workplans under the assumptions of the "Reduced Funding Scenario" presented in the MCC renewal bid, subject to further consultation with the MCC committee.

CRYSTAL: The support we will provide to MCC will be in the form of new developments, code performance improvements of the recently released CRYSTAL17 code, support to existing and new users and collaborations on scientific project of interest to MCC members and to STFC. Concerning the code development component, we will continue the work initiated in 2017-2018 concerning the extension of TD-DFT to systems involving electronic excitations to highly diffuse, conduction-like states in solids. This development will impact the ability of CRYSTAL to describe reliably the response of solids and other extended samples to wider ranges of radiations (from IR, to visible and UV, to X-rays). We will also work, in collaboration with the University of Turin (Italy) on an implementation of ab initio molecular dynamics (AIMD) in CRYSTAL. In addition, we will complete a new hybrid OpenMP-MPI version of the code (in collaboration with Oxford University), which also involves major restructuring of several core routines in the code. We are currently involved in a number of scientific collaborations with UK universities and STFC experimental Facilities in the fields of catalysis, excited states and optical spectroscopy, low-dimensional systems and the simulation of vibrational properties of material.

ChemShell: ChemShell development will continue to focus on the new Py-ChemShell code. 0.1 FTE continues to be committed to supervision of the ChemShell work packages in the MCC flagship software development project "SAINT". There is interest in further QM code interfaces in Py-ChemShell for embedded cluster calculations, for which we judge the ORCA code to be the highest priority. We will improve usability of the code for reaction path optimisations and enhance support for DFTB+ calculations through the development of a directly-linked interface for HPC platforms. Py-ChemShell will be installed and supported on ARCHER and Tier 2 systems such as UCL's Thomas facility, and maintenance of the legacy codes Tcl-ChemShell and GAMESS-UK will continue throughout the reporting period.

DL_POLY: Collaborative support (Kostya Trachenko @ QMUL, Alexey Sokol @ UCL) and provision of training and outreach in assistance with other CoSeC partners (CCP5, CCPBioSim, UKCOMES) will continue on an ongoing basis. Support to CCP5 Summer School and outreach events will be provided as lectures on Molecular Dynamics and demonstration of capabilities of the project. Supervision and personnel develop effort will focus on code learning with the major aim at refactoring due to a number of large development efforts; CCP5 supported Empirical Valence Bond (EVB) and Shaped Particles (SHP) as well as EPSRC eInfrastructure supported Density Functional Tight Binding (DFTB) and Forward Flux Sampling (FFS). The work will also include mapping, new coverage test cases, performance scaling recording, new user relevant and EVB and SHP project webpages.

DL_FIELD: More new features relate to inorganic materials will be introduced in order to improve flexibilities and automation processes of setting up inorganic models. Some form of automation of

setting up mixed parameters will be implemented between the inorganic and organic components. In addition, CWY has demonstrated DL_FIELD/DL_POLY capabilities and secure a collaborative work with the University of Manchester to run large-scale simulations of graphene-cellulose nanocomposites for lightweight electronic devices. Such models cannot directly implement in some traditional bio-packages such as AMBER. The bio-inorganic features and the project-driven software development effort will also be translated to study cases and demonstrations in the future DL_Software training courses.

Staffing	**Effort**
Leonardo Bernasconi	1.00 FTE
~~Barry Searle~~	~~0.22 FTE~~
Ilian Todorov	~~0.75~~ 0.46 FTE
Chin Yong	0.23 FTE
Tom Keal	~~0.50~~ 0.10 FTE
~~ChemShell Developer~~ David Gunn	~~0.40~~ 0.36 FTE
Total	**~~2.47~~ 2.15 FTE**

NB: Table updates reflect the reduction in SLA support to MCC from 2.5 FTE to 2.0 FTE from November 2018. Staff effort given below follows the assumptions of the 'Reduced Funding Scenario' presented in the MCC renewal bid, but is subject to further discussion/confirmation with the MCC committee.

MCC – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

We will continue to follow the SLA plans outlined in the MCC renewal bid under the constraints of the reduced funding awarded, subject to ongoing review with the MCC committee. Our planned targets for Py-ChemShell include the extension of the subtractive periodic QM/MM scheme to CASTEP and methods for multiple electronic states (conical instersections and surface hopping dynamics). DL_POLY and DL_FIELD targets include the calculation of thermoelectric coefficients via equilibrium MD, code refactoring in preparation for python interfaces, and inclusion of features for organic-inorganic interfaces. In CRYSTAL the extension of the TD-DFT code to conduction-like excited states will be concluded and work planned to begin on force and density matrix propagation in ab initio molecular dynamics.

UKCP – UK Car-Parrinello Consortium

The United Kingdom Car-Parrinello Consortium (UKCP) is a group of researchers across the UK who develop `first principles' quantum mechanical techniques for studying atomistic systems and apply them to a very wide variety of systems. The UKCP consortium is one of the longest-running High-End Computing Consortia in the UK, and has been funded almost continuously by EPSRC since the 1990s. The 1 FTE of core support is currently focused on supporting the CASTEP code, one of the UK flagship first principles codes.

UKCP – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Plans for the 2017/18 period cover consolidation of recent work, community outreach, software maintenance and new code development. In direct support of the UKCP and wider CASTEP community, the annual CASTEP software release management, teaching workshop and code developer's workshop will be carried out. The DFPT Raman project will benefit from code optimisation and post-processing tools, which will further improve the time to science for users simulating Raman spectroscopy. The Jenkins continuous integration system will be brought into production for CASTEP development work. This will allow CASTEP developers to efficiently test their code in a large number of computer system configurations. We plan to produce a specification of Python-based post-processing tools for CASTEP, this will improve the maintainability of the post-processing tools going forward, reducing bugs for users. We will also trial an electronic software licence management system

for academic CASTEP, superseding the existing physical paper forms used until now. In terms of new code development, we plan to apply Stewart Clark's (Durham University) "Local Fock Exchange" to the construction of pseudopotentials. This would be a novel approach to include non-local physics in the approximation of a frozen set of core electrons within simulated atoms.

UKCP	Milestone	Target Date
	Consolidation of CASTEP's Raman and NLO "2n+1" code: including symmetry, calculation checkpoints, optimisation, and post-processing tools Ongoing – some of the above to be released as part of CASTEP 19.1	~~Q2 2017~~ Q4 2017
	Produce specification for post-processing tools based on the CASTEP Python interface Discussion held with Phil Hasnip. Plans for 2018/19 updated to implement first tool based on the Python interface.	~~Q2 2017~~ Q3 2017
	Bring SESC's Jenkins CI system into production for CASTEP, superseding buildbot Complete	Q3 2017
	Co-organization and teaching of CASTEP workshop in Oxford Complete. This was a very successful event	Q3 2017
	Organisation of 2018 CASTEP "codefest" core developer workshop Complete	Q4 2017
	Trial and produce an electronic license management system for academic CASTEP STFC is to use the e-lucid license management system. CASTEP will be one of the pilot projects to use the system when it is in place (estimated Q3 2018)	Q4 2017
	Release management of CASTEP 18 including documentation and liaison with major HPC services Complete	Q4 2017
	Code CASTEP on-the-fly pseudopotentials for exact exchange based on Stewart Clark's "Local Fock Exchange" Further discussion has taken place with Stewart Clark and CASTEP developers. This work is ongoing and will coordinate with Stewart Clark in preparation for release of the OEP/LFX functionality in CASTEP main. Lower priority task for Q2 2019.	~~Q1 2018~~ Q2 2019

Staffing	Effort
Dominik Jochym	1.00 FTE
Total	**1.00 FTE**

UKCP – Summary Report (1 April 2017 – 31 March 2018)

Dominik Jochym organised the annual CASTEP core developer workshop "Codefest", which was very successful, with positive feedback received from the participants. The focus of this year's meeting was to consolidate the regression test suite (users receive a higher quality, more reliable product) and to continue low level module refactoring. These activities are essential to the continued longevity of the CASTEP project and enable future development opportunities such as a deep Python interface to CASTEP.

A bug fix release of CASTEP, v17.2.1 was made available in July 2017. A new major version of CASTEP is on track for release in December 2017. Much of the reliability of the v18.1 release is a direct result of the Jenkins Continuous Integration (CI) system that has been brought into production. CI enables

automated compilation and testing of software, and hence increases the productivity of developers and reduces the number of software problems for end users. The Jenkins scripts that are used for the CASTEP project are available on request.

The annual joint UKCP/CCP-NC CASTEP workshop continues to be a success with Dominik Jochym contributing to the event through delivery of training material. Concurrent with the user workshop, a code development workshop was held for 8 participants that focussed on how to contribute code to CASTEP. Dominik Jochym assisted with delivery of training material, including best practice and software development tools such as version control, unit and regression tests, continuous integration and code specification. This activity ensures that contributions to CASTEP have a path to be included in official releases and disseminates essential skills for future leaders of software development projects.

Dominik Jochym attended the annual RSE conference and, with Joseph Parker (CCP/HEC-Plasma), represented CoSeC staff from STFC-RAL at the ARCHER 2 town hall. This activity presented an opportunity to represent the needs of CoSeC staff to better support our communities on the next generation of national compute service.

Dominik Jochym has been in discussions with STFC Business Innovation Directorate, Legal and Finance to represent CASTEP as a potential pilot for the use of the e-Lucid system. The platform provides license management and electronic media distribution, which will become a key part of STFC's distribution of software. Input represented the interests and requirements of UKCP in the wider context of the varied licenses used by CoSeC supported software. STFC will be bringing the platform into production in 2018.

To widen the impact of CASTEP, Dominik Jochym has taken up roles supervising and leading projects to aid the STFC ISIS Neutron and Muon Facility in the use of simulation to interpret experimental data. In conjunction with Simone Sturniolo (CCP-NC) and Leandro Liborio (STFC-SCD) we have developed a general purpose approach and prototype user tool for the determination of Muon stopping sites. The initial implementation made use of CASTEP and has been extended to Quantum Espresso and DFTB+ with support for more codes planned through the Atomic Simulation Environment.
The PACE project (Proper Analysis of Coherent Excitations) has been funded by STFC-ISIS as a software development project in lieu of an instrument upgrade. The aim is to develop a suite of tools around Toby Perring's (STFC-ISIS) HORACE code to greatly improve the capabilities of analysing, modelling and fitting dynamical structure factors. Dominik Jochym's role in this includes advice on distributed computing, production of quality software to users and bridging the gap between simulated atomic vibrations and experimental measurements. Supervision and one-to-one CASTEP training of Rebecca Fair (STFC-SCD), who is developing code for PACE, is an additional responsibility of this role.

Albert Bartok-Partay has produced new code in CASTEP to improve the underlying approximations used by DFT. From January 2018, this work is 20% under UKCP and 80% CCP-NC. The ability for CASTEP to use "meta-GGA" levels of approximation will positively impact both UKCP and CCP-NC communities and reflects division of labour from Dominik Jochym on CASTEP projects with STFC facilities.

UKCP – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

Plans for the 2018/19 period cover consolidation of recent work, community outreach, software maintenance and new code development. In direct support of the UKCP and wider CASTEP community, the annual CASTEP software release management, teaching workshop and code developers workshop will be carried out. The DFPT project for Raman and non-linear optics will be expended to compute phonon lifetimes. This will allow improved use of Boltzman Transport Equation

codes that interface with CASTEP used for the simulation of properties such as thermal conductivity. The Jenkins continuous integration system will be extended to test environments on high performance computing facilities such as Archer and Thomas. This will allow CASTEP developers to efficiently test their code in the same environment that is used for production CASTEP calculations. We plan to re-write the existing tool for electron and phonon dispersion to build on the specification of Python-based post-processing tools for CASTEP. This will improve time to science for a large subset of CASTEP users. The genetic algorithm (GA) approach to solve the crystal structure problem has been in the development pipeline for CASTEP for many years. We plan to prepare the existing code for release alongside a case study to apply the GA code. Finally, we plan to implement van der Waals DFT functional in the style of Dion et al. This will lead to the availability of a number of vdW-DFT functionals in CASTEP, which will improve the modelling of systems that require precise description of intra-molecular forces, e.g. pharmaceuticals.

Work on the Tran-Blaha exchange potential implementation in CASTEP that was started in 2016, and is currently in alpha testing phase, will be finished. A paper discussing the implementation details and questions about pseudopotential generation is also planned. Building on the Tran-Blaha work, implementation of the state-of-the-art meta-GGA functionals is planned which will bring improved accuracy for a wide range of atomistic systems.

Staffing	**Effort**
Dominik Jochym	~~1.00~~ 0.80 FTE
Albert Bartok-Partay	0.20 FTE
Total	**1.00 FTE**

UKCP – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

In direct support of the UKCP and wider CASTEP community, the annual CASTEP software release management, teaching workshop and code developer's workshop will be carried out. New code development will continue to extend the capabilities of the exchange correlation functionals planned for 2018/19.

UK-COMES - UK Consortium on Mesoscale Engineering Sciences

The United Kingdom Consortium On Mesoscale Engineering Sciences (UKCOMES) – founded in 2013 – is a group of researchers across the UK who develop and apply mesoscopic modelling techniques to explore systems of scientific and industrial interest at scales between atomistic and continuum-based levels. Several modelling techniques are applied in this consortium, but the most frequently used and studied is the Lattice Boltzmann Equation (LBE) method, a particle-based statistical technique capable of modelling fluid flows with complex geometries and interactions between multiple fluids and phases.

The 1 FTE of core support per year is focussed on developing DL_MESO, the consortium's community code for LBE simulations, by adding new functionality and optimising for various computing architectures. Both activities allow for a wider range of systems to be modelled with available computing resources, including the UK's national supercomputer ARCHER.

UK-COMES – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Two new features will be added to DL_MESO's LBE code over the coming year. Schemes to apply immersed boundary conditions will be added to allow modelling of deformable objects in fluid flows, as will implementations of contact angle hysteresis to more accurately model advancing and receding effects of droplets moving along surfaces.

A new LBE code based on using the Oxford Parallel library for Structured-mesh solvers (OPS) will be documented and released, allowing automatic generation of optimised code for various hardware architectures, including Intel Xeon Phi and GPUs. A two-dimensional version of the code will initially be released and work will continue to extend it to three-dimensional systems. This code is based on prior work by Jianping Meng and is designed to be a prototype for re-engineering DL_MESO with the planned High-Level Mesoscale Modelling System (HiLEMMS); the project to create HiLEMMS is due to start in June 2017.

UK-COMES	Milestone	Target Date
	Prepare documentation of the OPS-based code for application developers Complete. Jianping currently looking at how to release the code	Q2 2017
	Implementation of immersed boundary method Postponed to Q2 2018 (see 2018/19 plans)	~~Q3 2017~~ Q2 2018
	Continue developing the OPS-based code; release a workable 2D version and start testing the 3D case. Postponed to Q2 2018 (see 2018/19 plans)	~~Q4 2017~~ Q2 2018
	Implementation of contact angle hysteresis In progress. May slip by a quarter. Postponed to Q2 2018 (see 2018/19 plans)	~~Q1 2018~~ Q2 2018

Staffing	Effort
Michael Seaton	0.45 FTE
Jianping Meng	0.55 FTE
Total	**1.00 FTE**

UK-COMES – Summary Report (1 April 2017 – 31 March 2018)

The work has been proceeding mostly as planned with support from Michael Seaton and Jianping Meng.

A new LBE code (MPLB) based on the Oxford Parallel library for Structured-mesh solvers (OPS) has been prepared for release to application developers by Jianping Meng. Code can be automatically generated and used for a wide range of hardware, including Intel Xeon Phi and GPUs via the support of various threading models. MPI can also be used to connect multiple accelerators, thus enabling large-scale numerical simulations for the UKCOMES community. This code will act as a prototype for the EPSRC-funded High-Level Mesoscale Modelling System (HiLEMMS) project, which involves developing a high-level coding abstraction for LBE simulations for automatic code generation.

The previously postponed task of implementing membrane dynamics in DL_MESO (from 2016/17) has been carried out between July and September 2017 as a summer project based at Sheffield Hallam University under Michael Seaton's supervision. This new functionality (currently limited to two dimensions but expandable to three) allows modelling of non-spherical drops as deformable fluid-filled vesicles, which can represent entities such as red blood cells. The same project additionally implemented continuum-based fluid/fluid interactions with large density contrasts in DL_MESO: this allows modelling of heavier drops or lighter bubbles in a background fluid with flows and minimal spurious flows from interfaces, which is ordinarily challenging for most LBE-based fluid/fluid interaction schemes.

UK-COMES – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

Two new features will be added to DL_MESO's LBE code over the coming year. Schemes to apply immersed boundary conditions will be added to allow modelling of deformable objects in flows. Modifications to the Lishchuk immiscible fluid algorithm in DL_MESO to allow large contrasts in density between fluids (working in collaboration with the Materials and Engineering Research Institute at Sheffield Hallam University) and to include larger numbers of non-coalescing drops will also be applied.

The new LBE code, MPLB, based on using the Oxford Parallel library for Structured-mesh solvers (OPS), will be extended to three-dimensional systems and tested using the Taylor-Green vortex, a common unsteady flow system with a known analytical solution used to test fluid flow solvers. The same code will also be extended to allow modelling of shallow water (free surface flow) equations with a newly-developed implementation of body forces for these types of flow. These will also be considered as example test problems for the High-Level Mesoscale Modelling System (HiLeMMS).

Staffing	**Effort**
Michael Seaton	0.45 FTE
Jianping Meng	0.55 FTE
Total	**1.00 FTE**

UK-COMES – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Newly developed viscoelastic models for lattice Boltzmann simulations will be added to DL_MESO's LBE code to compliment previously developed non-Newtonian rheological models and expand the types of fluid that can be modelled with this code. The same code will also be prepared for re-engineering along the lines of the High-Level Mesoscale Modelling System (HiLeMMS) and previous work to optimise DL_MESO for Intel Xeon Phi accelerators. The OPS-based code MPLB will be extended by adding turbulence models for higher speed problems and coupling the code to a finite-difference method solver for heat diffusion problems.

HEC Plasma Physics

HEC-Plasma and CCP-Plasma resources have been combined into a single workplan. Please see the report above under CCP-Plasma.

HECBioSim

HEC-BioSim exists to bring High-End Computing for biomolecular simulation to a wider community, including users from industry and experimental bioscientists, and to engage physical and computer scientists in biological applications. The Consortium works closely with CCP-BioSim.

HECBioSim is supported by 1.0 FTE of SLA core effort, which provides support for scientists applying for time on ARCHER, primarily through maintenance of the HECBioSim web portal. It includes help on preparation of applications e.g. with the HECtime resource calculator, and on reporting the outcomes of approved projects. The SLA post also works on a variety of codes for biomolecular simulation and analysis appropriate to High End Computing. For further information please see www.hecbiosim.ac.uk.

HECBioSim – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

Specific plans for this year are:

1. A comprehensive benchmarking study of MD codes across a selection of machine architectures (ARCHER, GPU, Xeon Phi). This activity produces data relating to the performance profile of a given code on a given machine. This data can then be used by applicants for time on e.g. ARCHER to justify the size of their resource requests. The consortium resource allocation panel can also make use of such a tool to assist with screening applications for time on ARCHER. In this reporting

period, data from machines other than ARCHER will allow us to provide data for machines with GPU's or Intel Xeon Phi co-processors thus allowing researchers to get an idea of which machines are most suited to their simulations. The following milestones are proposed:

a. Compilation of the latest MD codes on a number of machines (often the latest codes are not available). The benchmarking suite could be extended to include DESMOND and DL_POLY for performance comparison and potentially extend our list of supported codes.
b. Collect data from the benchmark suite.
c. Generate a predictive model based on the benchmarking data to allow performance predictions to be made.
d. Wrap the model in a new GUI that will be available through the HECBioSim website to allow users to see which hardware would most suit their simulation type/size etc. The ARCHER specific data should also be included into the current ARCHER time calculator tool.

2. On-going maintenance of the HECBioSim and CCPBioSim webpages. This includes server maintenance, backups, software upgrades and responding to cyber security related threats. Also part of this work the modification webpages of both websites based on information from last management meeting will be conducted and will include:

   HECBioSim – Changes to this site are related to changing the application forms to reflect change in collection of information. Applicant guidance material should be modified to include more information about what to put in a technical case. A new section for releasing the consortia annual reports, and a new section for publishing high quality case studies to showcase some of the research that the consortium supports.

   CCPBioSim – Changes to this site are related to changing the events system to make sure historical events are prominent and to also make the entry and prominent display of delegate feedback possible.

3. Provide technical support and assistance to Sarah Harris at Leeds with producing the research highlights for the CCPBioSim website. The research highlights are a concerted effort to develop a structured way to promote the incredible work undertaken by the community. This project will focus on developing the necessary skills and methods for producing high quality highlights.

4. Longbow is now a stable release, however ongoing support for its development will include the following:
   a. Re-license Longbow to a more permissive licence, the GPLv2 license harms certain types of developments that might wish to use Longbow. A consultation needs to be done with developers/users as to the best license.
   b. Release version 1.5.0, which will be under the new license chosen in 6.1. This release will include:
      i. Fixes for two bugs that lead to bad crashes.
      ii. Introduce friendly naming format for jobs/recovery files.
      iii. Introduce automated cleanup of old recovery files.
      iv. Introduce better importing for developers.
      v. Remove capitalisation of Longbow throughout codebase (source of major annoyance to developers)
      vi. New documentation for developers, i.e. an integration guide
   c. Support other project developers with Longbow integrations, such as integration with FESetup, ChemShell, Melody.
   d. Develop further cross CCP/HEC consortia links with regards to collaborative use and development of the Longbow tool.

5. Investigate the possibility of proceeding with Crossbow (the cloud tools variant of Longbow) development with Charlie Laughton at Nottingham University.

6. Investigate the viability of the Force Field Validation project with Francesco Gervasio at UCL.

7. Investigate supporting Sarah Harris at Leeds with porting their finite element based biosimulation software for large systems to ARCHER. The code currently uses OpenMP directives for parallelization. This code will need to be modified to use MPI before it can be compatible with ARCHER.

8. Promote HECBioSim and Longbow at meetings, for example at the CCPBioSim annual meetings.

HECBioSim	Milestone	Target Date
	Webpage modifications Complete	Q2 2017
	Benchmarking study with webapplet for data Complete	Q3 2017
	Deliver Longbow version 1.5.0 (4.2 above) Complete – issued end of June.	Q3 2017
	Chemshell – Longbow integration Complete	Q4 2017
	~~3 research highlights~~ ~~Plan in place for the first 2 highlights – (FFEA) one about optimisation to run on ARCHER on one with CCPEM.~~ Establish the Training section of the website Complete (moved forward from 2018/19 due to training workshop in April 2018)	Q1 2018

Staffing	Effort
James Gebbie	1.00 FTE
Total	**1.00 FTE**

HECBioSim – Summary Report (1 April 2017 – 31 March 2018)

James Gebbie-Rayet provides full time support for the HECBioSim project.

A number of changes to the HECBioSim website have been completed. The ARCHER time application form was modified to make the collection of applications into research “themes” possible. A section was created for the HECBioSim annual reports, and the 2016-17 year report was translated into HTML for inclusion. A new section for case studies was added, and the three case studies from the 2016-17 annual report were included, the aim of this is to increase the visibility of the high-quality research enabled by the HEC consortium in a visually appealing manner.

Longbow is the light-weight simulation submission engine developed in a collaboration between James (STFC) and Charlie Laughton (Nottingham). Longbow functions to seamlessly offload simulations to powerful super computers in a manner that appears to the user as the simulation had run on their own PC. Longbow handles all file transfer, scheduling, monitoring and is capable of doing complex multimachine submission patterns. Currently Longbow has been downloaded 5,202 times. Longbow developments during this period have focused around the release of version 1.5.0, which focused on fixing issues reported by users and is summarised under Major Code Developments.

Longbow continues to be used as a job submission system under the hood of the CCP-EM toolkit FLEX-EM. Two Hartree Centre projects are working to include Longbow in their code base, one aimed at automated compilation, and runtime performance optimisation and tuning. The other is a biosimulation setup, launch and analysis workflow tool. Further Longbow integration projects are being planned.

Benchmarking produces performance data vs simulation size and is delivered to both the community and our HEC resource panel in the form of an online calculator applet, such that improved estimates of the level of ARCHER time required for project applications can be made. This leads to less under-used time allocations per project and allows the resource pool to fund more projects.

The benchmark suite has been modernised to work with the latest versions of AMBER, GROMACS, LAMMPS and NAMD. The input files that the benchmark suite comprised of had compatibility issues with the latest versions of each code, mostly due to deprecated features and new methods. These problems had to be on a code by code basis iterated out and reparametrised with the current best practice parameters. These new benchmarks have now been packaged into a suite with some Python tools for launching (via Longbow) and processing of the data.

Benchmarking data has currently been collected for GROMACS 5.1.4 and 2016.3, NAMD 2.12, LAMMPS 17.11.2016 and AMBER 16. These benchmarks are now used to help inform users on the state of the art performance of these codes on ARCHER and to directly feed into their applications for consortia time.

Chemshell is a popular tool for setting up and performing Quantum Mechanical calculations developed by the MCC and CCP5 consortia with strong support for biomolecular QM/MM simulations. The newest version of Chemshell has been modernised to include a python interface. It is thus natural that both the biosimulation and materials community would benefit from the simplicity delivered by Longbow-Chemshell integration. In this reporting period, Longbow and the new Chemshell have been integrated such that Longbow can now fully support the vast array of use cases that Chemshell offers. This is both convenient for the expert user but also brings with it a lower technical barrier for new or non-traditional users to HPC. New training opportunities have been identified where the two consortia can work together to offer training courses of the use of Chemshell and Longbow to do bio-simulation.

A new training resource has been made at www.ccpbiosim.ac.uk/training this is a front end to a new set of self-contained training modules. These training modules have been designed to plug the gap between what CCPBioSim offers at workshops and independent learning. These training modules are designed to allow more complex training programmes to be delivered than previously possible by building upon previous modules. All of these new modules are utilising modern methods of delivery such as jupyter notebooks and cloud provision to provide a seamless training experience for the user, with the source code collated on our github repositories to provide a single point source to update material going forward.

HECBioSim – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

HEC-BioSim exists to bring High-End Computing for biomolecular simulation to a wider community, including users from industry and experimental bioscientists, and to engage physical and computer scientists in biological applications. The Consortium works closely with CCP-BioSim.

The HECBioSim CoSeC post provides support for scientists applying for time on ARCHER, primarily through maintenance of the HECBioSim portal. This includes help on preparation of applications e.g. with the HECtime calculator, reporting the outcomes of approved projects, and maintaining the outreach webpages. The post also works on a variety of codes for biomolecular simulation and analysis appropriate to High End Computing. Specific plans for this year are:

1. On-going maintenance of the HECBioSim and CCPBioSim webpages. This includes server maintenance, backups, software upgrades and responding to cyber security related threats.

2. Create a new training section on the website for standalone web based training. Charlie Laughton (Nottingham) has taken responsibility for pushing other members into writing training in this format. Our role will be to establish the website pages with the tutorial materials tested by CCPBioSim CoSeC support.

3. Longbow, ongoing maintenance and implementation of fixes/solutions to community reported bugs and feature requests.

   a) Release version 1.5.1, this version will contain several bug fixes and will enable support for the NAMD SMP builds.

   b) Increase the number of example use examples in both the user documentation and developer documentation.

   c) Support other project developers with Longbow integrations.

   d) Develop further cross CCP/HEC consortia links with regards to collaborative use and development of the Longbow tool.

4. Integration of the FFEA code developed by the Sarah Harris group in Leeds with the CCP-EM software stack. This would greatly increase the user-friendliness of the code, in particular for manipulating volumetric data and producing smooth surfaces. The resulting code would form a platform for subsequent parallelization, enabling the code to run on ARCHER and other HPC machines and thus allow users to simulation large scale simulations.

5. A project to introduce community driven simulation metadata standards and to integrate those with webtools such as jupyter, github and slack to facilitate a standardised way of collecting, curating and collaborating with biosimulation data. As a demonstration of the power of Jupyter notebooks, we will prototype real-time monitoring of simulations via Longbow with a Jupyter front end, using the ChemShell QM/MM package as a test case.

6. Investigate future support for the development of Crossbow (the cloud tools variant of Longbow) and TioS (a web simulation platform) with Charlie Laughton at Nottingham University.

7. Promote HECBioSim and Longbow at meetings, for example at the CCPBioSim annual meetings.

Staffing	**Effort**
James Gebbie	1.00 FTE
Total	**1.00 FTE**

HECBioSim – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Plans for this year currently show that there will be tasks relating to the Jupyter metadata project and an increased level of involvement with BioSimSpace as it moves from initial development to longer term CoSeC based support. This will include further development and maintenance including the possibility of integrating Longbow into the workflow tool.

UK-AMOR

UK AMOR is a new High End Computing consortium which will work in the general area of AMO physics, using the 'R-matrix' methodology. The R-matrix method divides an energy-dependent scattering problem into a physically complicated but energy-independent inner region and a much simpler energy-dependent outer region. The method now solves the full electronic time-independent and time-dependent Schrodinger equations as needed. Problems studied using ARCHER will include:

a) The interaction of atoms and molecules with light including intense light sources. R-matrix with time-dependence (RMT) is the leading code in this area, allowing calculations at the intersection of atomic and strong-field physics. Ongoing extensions to molecules, and atoms in arbitrarily polarised laser

pulses will further establish the code on the world stage. This will provide key support for exciting experimental work being performed on these physical processes.

b) Electron collisions with atoms, ions and molecules using UK codes which are widely used internationally. Calculations will focus on applications ranging from fusion plasmas to radiation damage in biological systems. For fusion we will focus on high accuracy calculations on atoms and ions, and key molecules important for fusion experiments. The consortium will also perform high accuracy electron-molecule collisions calculations to study:

1. *large systems such as molecular clusters and biomolecules where results are important for studies radiation of tracks and DNA damage.*
2. *processes of applied relevance for extended energy ranges,*
3. *processes of applied where improved models will provide more accurate scattering data*
4. *benchmark problems with full uncertainty quantification.*

These studies are only possible using the new UKRMol(+) code and ARCHER.

c) Ultracold chemistry: this a new area of study. Codes will be developed to treat ultraslow collisions for reactive systems over deep potential wells. Such systems are characterised by complex resonance structures whose study offers unique opportunities for chemical control and insights into this fundamental process. The methodology will also be applicable to a variety of related low-energy processes such as radiative association. Calculations will be performed on systems accessible to planned state-of-the-art experiment.

UK-AMOR – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

UK-AMOR has 0.2FTE dedicated CoSeC support plus some general support administrative and scientific support by Martin Plummer as part of CCPQ's CoSeC support allocation (described in the CCPQ plans, as are MP's plans to use some UK-AMOR Archer time to carry out test 'double-continuum' calculations of atomic electrons in ionizing collisions and laser pulse interactions) . The UK-AMOR membership comes from the CCPQ community. The management committee includes leading researchers in UK-AMOR's themes and CoSeC representation (MP). The initial CoSeC support request request was for Andrew Sunderland to perform various software development tasks and for SEG members to continue curation tasks (SESC Build Service /ANVIL) for the RMT codes, currently funded via CCPQ's Flagship Project, in the 2nd half of the UK-AMOR project. With a limited 0.2FTE allocated, AGS will supply this support for the first two years of UK-AMOR, with a focus on further adapting collision code PFARM (see the CCPQ report and plans) for the new ultra-cold chemistry package RMAT_REACT, to treat ultracold molecule-molecule resonances. The main, separate RMAT_REACT development will be performed by the UK-AMOR PDRA at UCL.

Staffing	**Effort**
Andrew Sunderland	0.20 FTE

UK-AMOR – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

The plans for direct UK-AMOR CoSeC support for 2019-2020 will follow on directly from the 2018-2019 work, continuing the outlined development of the resonance characterization package (the completed package would then be used for ultracold molecules work and fed back into the electron-molecule package UKRMol(+)). This is a result of the limited time (0.2FTE) allocated for direct UK-AMOR support. MP will continue to support UK-AMOR separately as part of CCPQ support plans.

UKTC - The UK Turbulence Consortium

The UK Turbulence Consortium brings together complementary expertise/experience/knowledge and coordinate activities to look at coherent, rational and strategic ways of understanding, predicting and controlling turbulent flows using High Performance Computing. The consortium is crucial for the UK in order to coordinate, augment and unify the research efforts of its participants and to communicate its expertise and findings to a wider audience.

UKTC – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

UKTC will start on 30th June 2018 with the intial task of investigating Lagrangian particle transport at scale using the Code_Saturne software.

Staffing	Effort
X Gu	0.30 FTE

UKTC – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Investigate the feasibility of implementing Lagrangian transport modules in Code_Saturne into another UKTC code.

UKCTRF - UK Consortium on Turbulent Reacting Flows

The new expanded UK Consortium on Turbulent Reacting Flows (UKCTRF) will further utilise the developments of High-Performance Computing (HPC) to offer improved fundamental understanding and modelling of turbulent reacting flows, which are pivotal in the effective usage of energy resources, development of reliable fire safety measures, and manipulation of the combustion processes to ensure environmental friendliness.

UKCTRF – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

UKCTRF will start in January 2019 with the intial task of assessing the status of the HAMISH development on ARCHER.

Staffing	Effort
Jian Fang	0.13 FTE

UKCTRF – 2019 / 20 Outline Plans (1 April 2019 – 31 March 2020)

Integrating development from the Software for the Future project into HAMISH and comparing with SENGA+..

Software Outlook

Software Outlook focuses on software technologies that are vitally important to the development and optimisation of the world-leading scientific software produced by the CCPs. This includes evaluation of new programming techniques that are essential for the timely and cost-effective exploitation of current

and near-future High Performance Computing systems, and demonstrating how specific software technologies can be applied to existing applications.

Software Outlook – 2017 / 18 Plans (1 April 2017 – 31 March 2018)

In 2017/18, we plan to continue our work investigating the use of mixed-precision within CCP codes. In particular, we will be considering codes from CCP5 and CCP-Plasma. To enable the CCPs to independently deploy mixed-precision within their codes in an effective manner, we will develop a general framework for its use and provide training to the CCPs (web-based training and the provision of workshops at CCP meetings).

We will also continue our code-coupling effort and will work closely with CCP-WSI to identify bottlenecks and improve the coupling methods used to give better performance on HPC platforms.

Collectively, the CCPs provide a large number of software packages to their users and information about these packages is scattered across different websites and in various journals. We will perform an audit of these software packages, gathering information from the CCPs on a number of metrics such as the type of software license, support available, and performance of the code on HPC provisions.

Software Outlook	Milestone	Target Date
	CCP5's use of mixed-precision within DL_MESO (CCP5), in which Michael Seaton has a specific request to look into splitting a particular DP measurement into two contributions A+B, where A is large (relative to B) and unchanging, and B is continuously modified but should be able to be calculated in SP and stored in SP. Removed. Following further reduced precision experiments in DL_POLY, this was dropped in favour of extending the remit of the training package. The DL_POLY experiments also implied that the DL_MESO proposal was unlikely to yield good enough savings in execution time	~~Q2 2017~~ Q3 2017
	Coupling Type 1: Simplest Case: OpenFOAM-to-OpenFOAM coupling. How is the coupling done in Floating Buoy test example? Does it scale well? What percentage of time is spent doing the coupling. Investigate reason for general OpenFOAM scaling problems for this problem Complete. Andrew Taylor was able to get an extensive amount of data, which is going to form the basis of a joint paper between Andrew and Ed Ransley	~~Q2 2017~~ Q3 2017
	Work packet revolving around FLAME from CCP-Plasma Removed. Dropped in favour of the expanded mixed precision training package.	~~Q3 2017~~ Q4 2017
	Development of a more general framework to guide the CCPs in deciding whether mixed-precision would be a valuable attribute to their codes. This would involve the production of written training material as well as the possibility of a webinar. Ongoing. In the final stages of producing the training package. Some of the webinars have been recorded. Will move to 2018/19 plans	Q4 2017
	Investigating the effects of using mixed-precision approaches on novel architectures available within the Hartree Centre Removed. Problems with the Hartree computing infrastructure meant that this was not possible	Q1 2018
	Coupling Type 2: Boundary between two regions: OpenFOAM-to-OpenFOAM coupling. How can this coupling/communication be done in an efficient manner, which scales well? Load balancing	Q1 2018

	during the simulation is terrible. How can it be improved? Test examples to be provided by CCP-WSI CCP-WSI were unable to provide us with the required test problem due to staffing shortages. This was replaced by extending the remit of the TAU training package	
	Software Audit of CCP Software Audit sent out mid-December. Deadline extended from end-Jan to end-Feb. Work package suggestions used in 2018-19 work plans. Full analysis to be done in Q2 2018 due to extended submission deadline	Q1 2018

Staffing	**Effort**
Luke Mason	0.40 FTE
Sue Thorne	0.60 FTE
Andrew Taylor	0.79 FTE
Total	**1.79 FTE**

Software Outlook – Summary Report (1 April 2017 – 31 March 2018)

During this reporting period, Software Outlook has been working on the code coupling, mixed-precision coding and software audit work packages. The code coupling and mixed-precision work packages were extensions of work packages from the 2016/17 period but the software audit is completely new to Software Outlook.

Code Coupling for Multi-physics and Multi-scale CFD Applications

The coupling of two independent applications is a common requirement by a number of the CCPs, for example, CCP_WSI. However, the coupler is often found to be a bottleneck when the codes are run using 100+ processors or cores. CCP-WSI are reliant on code coupling within their simulations and Software Outlook has been collaborating with them to investigate how to ensure that the coupling does not become a bottleneck for their particular type of problems. The first test problem provided by CCP-WSI uses OpenFOAM to simulate a floating buoy: the parallel scaling is poor and we have been investigating the cause of this. As part of this investigation, we had to link TAU, an open source performance profiler, to OpenFOAM. TAU has a large range of functionalities but, through the combination of poor documentation and the highly complicated nature of OpenFOAM, getting the profiler and OpenFOAM to work together was a challenge. Once we got them to work in unison, it was then difficult to extract useful information because of the nature of the large test problems. However, we have been successful in doing this and have developed a comprehensive training course to help other software developers suceesfully use TAU to profile their codes. The poor scalability of the test problem was found to be due to very bad load balance between the MPI processes. The outputs from this work were used by CCP-WSI and their partners in a successful eCSE grant bid. Andrew Taylor (Software Outlook) and Ed Ransley (CCP-WSI) are currently writing a journal paper using the results from this work package.

Mixed-precision and Power-Aware Computing within Scientific Applications

This work package has mainly focussed on the use of mixed-precision within CCP5's DL_POLY code. DL_POLY has turned out to be an excellent choice of code to use with mixed-precision because it has demonstrated when the code structure is or is not a good choice for trying mixed precision, and also demonstrated when it should or should not be used because of the underlying mathematics. In an average month of DL_POLY use on ARCHER, mixed-precision can save up to 80 (wall-clock) hours of computing time (450kAUs). This work was presented at two international conferences: 2nd Power-Aware Computing Workshop, 5-8th July in Germany, and 2nd Research Software Engineers Conference, 7-8th September in Manchester. We are in the final stages of developing a comprehensive training course on the use of mixed-precision within CCP/HEC codes. STFC's Hartree Centre offered us the use of their training course advisor and online provisions, which has allowed us to produce a far

more extensive training package. It was agreed with the Software Outlook Working Group that the extended training package should be our main deliverable and that we should concentrate on this instead of the DL_MESO and FLAME work.

Software Audit of CCP/HEC Codes
The software audit targetted the flagship CCP/HEC codes with the aim to establish whether they are "user-friendly" and "fit-for-future". For codes that are determined to need further development, our findings will help to inform bids for future work packages. The Software Audit was sent out to all CCP and HEC Consortia chairs in mid-December. The submission deadline was extended from the end of January to end February following requests from the community. As a result, a full analysis has not been completed but the work package suggestions were used to inform our 2018-19 Work Plan. There were a total of 36 responses to the audit.

Software Outlook – 2018 / 19 Plans (1 April 2018 – 31 March 2019)

(Detailed plans and milestones are included in Appendix 1 for reference)

The Software Outlook activity focuses on software technologies that are vitally important to the development and optimization of world-leading scientific software. This includes evaluation of new software technologies, e.g. programming languages, libraries and techniques, that are essential for the timely and cost-effective exploitation of current and near-future systems and demonstrating how specific software technologies can be applied to existing applications.

Hybrid Programming with GPUs and CPUs
During the last 10 years, the use of CPUs in conjunction with GPUs has gone from being an interesting research idea (with institutions purchasing standalone systems with GPU cards to investigate their use) to recent HPC clusters having large numbers of GPUs. Thus, hybrid GPU/CPU possibilities are now widely available and frameworks/libraries for using them have rapidly evolved. Many CCPs and HECs are now wanting to exploit these next generation architectures and wish to appropriately port their simulation codes. A survey of hybrid programming frameworks will be done and comparisons of GPU support will be performed using suitable kernels from CCP codes. We will also provide training on porting codes, including when it is suitable to do this and when it should be avoided. As well as GPUs, other accelerators will also be considered.
Planned effort: 0.7 FTE

Physics and Mathematics Libraries
Physics and mathematics are at the heart of most simulation codes. There are normally parts of the code where external physics and maths libraries can be used and these parts of the code can quickly become a bottleneck if the wrong library or method is used.

Effective parallel linear algebra solvers with good parallel scaling properties are complex to code but frequently required in CCP codes. We will provide information and guidance on these libraries to meet the needs of the CCPs/HECs. For example, the developers of EPOCH (CCP-Plasma), want to add the ability to solve elliptic PDEs in a way that will scale acceptably to the processor counts that EPOCH needs to run on: only a small number of methods will be suitable. Additionally, a sub-optimal choice of method can also have a detrimental to other parts of the code. In BOUT++ (CCP-Plasma), the code is using time steps that are much smaller than they need to be because the convergence of the underlying iterative linear algebra method is so poor. By improving the convergence through more effective preconditioners, this will also enable the use of a larger time-step with the potential of dramatically improving the execution times and energy consumption values for these computational simulations.

Fast Fourier Transforms are another common kernel in CCP and HEC codes. The 2012 PRACE survey of FFT codes focussed on MPI codes. We will update the guidance from this survey and also consider

codes that use other parallelism methods to provide guidance to the software developers. For example, the developers of SIRF (CCP-PETMR) a suitable needing an OpenMP-based Fast Fourier Transform library that satisfies their license needs.

Staffing	**Effort**
Luke Mason	~~0.40~~ 0.20 FTE
Sue Thorne	0.60 FTE
Andrew Taylor	~~0.60~~ 0.20 FTE
Philippe Gambron	0.50 FTE
~~Xiaohu Guo~~	~~0.40 FTE~~
Total	~~**2.00**~~ **1.50 FTE**

Resource Planning and Yearly Costing

This section summarises the approach to resource allocation and yearly costing.

Level of funding and resource for the current SLA

During this cycle, a call for the HEC consortia will take place in 2017 and the total number of FTEs for the consortia is not expected to change from the current 5.7 FTE/year. A call for CCPs is also likely to take place in 2019. In the following considerations, we assume that the total number of FTEs for the CCPs will also not change, and that a drop by 2 FTEs in the level of funding will occur from the start of 2018/19. Under these assumptions, the total sum of the resource awarded to the projects is 113.00 FTEs.

In addition to delivering the full 113 FTEs of effort for the current 5 year SLA cycle, we have agreed that during this cycle we will make up for a shortfall in effort delivered that arose for several projects during the previous SLA cycle (up to 2015/16), as indicated in the table below. This historical shortfall was due to staff sickness and difficulties in recruiting suitable staff.

Summary table in FTE's of historical shortfall incurred during the previous SLA cycle (ended in 2015/16).

	Underspend up to 2014/15	Underspend during 2015/6	Carry over to 5 yr plan
Project Office etc	0.00	0.00	0.00
CCP5	0.32	0.10	0.42
CCP9	0.38	0.45	0.83
CCPmag	0.00	0.47	0.47
CCPNC	1.50	0.30	1.80
CCPQ	0.00	0.00	0.00
CCP Plasma	0.00	0.48	0.48
CCPi	0.00	0.33	0.33
CCPPetMR	0.00	0.33	0.33
CCP BioSim	0.00	0.00	0.00
MCC	0.00	0.00	0.00
UKCP	0.00	0.42	0.42
UK-COMES	0.00	0.00	0.00
HEC Plasma	0.00	0.00	0.00
HEC BioSim	0.50	0.00	0.50
Software Outlook	0.10	0.10	0.10
Totals	2.48	3.30	5.68

Planned Resource Profiles

In this current planning process, for each project we allow the amount of effort to vary from year to year and to be re-adjusted yearly as long as each project recovers its full support over the five years of the SLA cycle.

The following table shows the predicted spend profiling for the next five years. For 2016/17 and 2017/18 two figures are included – in **black**, the planned effort used to calculate the annual cost, and in **red** actual effort provided. For the HEC consortia yearly allocation, he figure in brakets shows the allocation

before the recent renewal. The figures in **pink** are the proposed figures for the remainder of the the current CoSeC SLA cycle.

	Agreed Carry Over	Yearly Alloc	2016-17	2017-18	2018-19	2019-20	2020-21	Total
Project Office	0.00	2.25	2.23 2.25	2.23 2.25	2.20 *1.45*	2.41 *1.40*	2.37 *1.33*	**11.25** ***8.64***
CCP5	0.42	3.20	1.95 2.82	3.19 3.56	3.94 *3.68*	3.27 *4.10*	4.23 *3.18*	**16.42** ***16.10***
CCP9	0.83	2.40	2.64 2.71	2.28 2.70	2.86 *2.90*	2.67 *2.68*	2.45 *2.33*	**12.83**
CCPmag	0.47	0.74	0.64 0.83	0.70 0.40	1.23 *1.23*	1.15 *1.05*	0.74 *0.55*	**4.17**
CCPNC	1.80	1.30	1.62 1.50	2.00 2.00	1.80	1.10 *1.59*	1.80 *1.29*	**8.30**
CCPQ	0.00	1.86	1.69 1.86	1.80 1.86	2.00	2.06 *1.99*	1.86 *1.82*	**9.30**
CCP Plasma	0.48	0.75	0.79 1.00	0.79 0.80	0.80	0.83 *0.80*	1.04 *0.80*	**4.23** ***3.97***
CCPi	0.33	1.20	0.82 1.45	1.01 1.50	1.56 *1.35*	1.63 *1.70*	1.29 *1.20*	**6.33** ***6.09***
CCPPetMR	0.33	1.20	1.09 1.15	1.53 1.50	1.44 *1.40*	1.02 *1.08*	1.20 *1.23*	**6.33**
CCPBioSim	0.00	1.20	1.19 1.16	0.79 1.20	1.20	1.27 *1.20*	1.60 *1.18*	**6.00** ***5.56***
MCC	0.00	(2.50) 2	2.53 2.50	2.32 2.50	2.75 *2.15*	2.41 *2.00*	2.50 *1.99*	**(12.50)** **11.15** ***10.99***
UKCP	0.42	1.00	1.36 1.42	0.97 1.00	1.00	1.14 *1.20*	1.00 *0.74*	**5.42** ***5.27***
UK-COMES	0.00	(1.00) 0.6	0.93 1.00	1.16 1.00	1.00 *0.60*	0.92 *0.59*	1.00 *0.59*	**(5.00)** **3.87**
HEC Plasma	0.00	0.20	0.20 0.20	0.20 0.20	0.20	0.20	0.20	**1.00**

HECBioSim	0.50	(1.00) 0.8	0.98 1.00	1.01 1.00	1.00	1.25 *1.00*	1.26 *1.01*	**(5.50)** **5.00**
UK Turbulence	0.00	(0) 0.40	0.00	0.00	0.30	0.40	0.40	**1.10**
UKCTRF	0.00	(0) 0.50	0.00	0.00	0.13	0.50	0.50	**1.13**
UKAMOR	0.00	(N/A) 0.20	0.00	0.00	0.20	0.20	0.20	**0.60**
Software Outlook	0.10	2.00	2.31 2.00	1.64 2.00	0.00 *1.50*	0.00 *1.50*	0.00 *1.48*	**4.10** ***8.43***
FTE TOTALS	**5.68**	**24.90**	**22.97** **24.86**	**23.62** **24.66**	**24.75** ***24.89***	**24.01** ***25.18***	**22.29** ***22.02***	**118.68** ***118.68***

Planned vs Actual Resource

While the resource planning is now done over a 5-year period, the costing of the programme needs to be calculated on a yearly basis based on the planned effort. Deviations between planned and actual effort are calculated and used to reprofile the effort and costing for future years. For both 2016/17 and 2017/18, the difference between delivered and planned effort for each project has been calculated and redistributed over future years so that by the end of the SLA cycle each project will spend the amount of FTEs awarded for this SLA plus any historical underspend that a project may have incurred.

2018/19 Planned Resource and Costing

Of the planned 24.89 FTEs for 2018/19, 21.74 FTEs have been costed via the SLA, while 3.15 FTEs will be provided based on funding received previously (i.e. carry-over from previous SLA or adjustment due to deviation between planned and actual effort). The detailed cost breakdown for 2018/19 for the 21.74 FTEs is as follows:

Please note that recurrent expenditure includes:

- Travel and Subsistence – this includes T&S for our staff attending management/ project meetings. Includes T&S for visitors.

- Consumables – includes items such as telephone charges, training, photo repro, registration fees and workshop costs.
- HW/SW – this includes capital purchase of desktop/ laptop systems, software maintenance and applications packages.
- Participation in Supercomputing, production of annual report and general support activities around the SLA including the web.
- Hardware and software maintenance costs.
- Computing Infrastructure covers maintenance of servers, software licenses and printing consumables. Staff effort supports hardware and software maintenance and systems management of desktop systems and fileservers and support of visualisation and grid infrastructure.

Metrics

The metrics currently used for this programme are defined as:

- Number of citations in peer-reviewed journals of a publication about software supported by SLA-funded staff. **Please note that not all software packages we support have a citeable publication.**
- Number of training days delivered by SLA-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 by SLA funded staff.
- Number of scientific/technical presentations at external events delivered by SLA-funded staff.

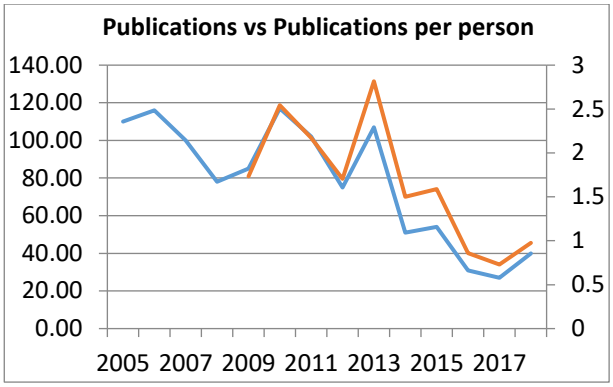
The metrics are per financial year, with the exception of the citations metric, which is for calendar year (for ease of data collection). Please note that for an interim report the data collection for the current year is partial for all metrics except the citations.

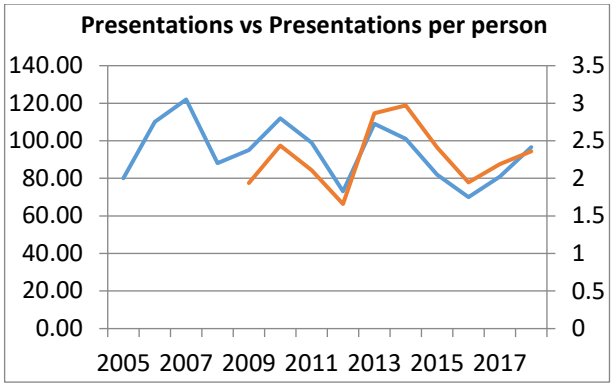
In the metrics graphs below, the blue line refers to the total number while the red line refers to the number per scientific/technical staff member. This is useful because metrics are included for any person irrespective of whether they are partially or fully funded by the SLA. For information, a graph of the scientific/technical staff headcount has also been included.

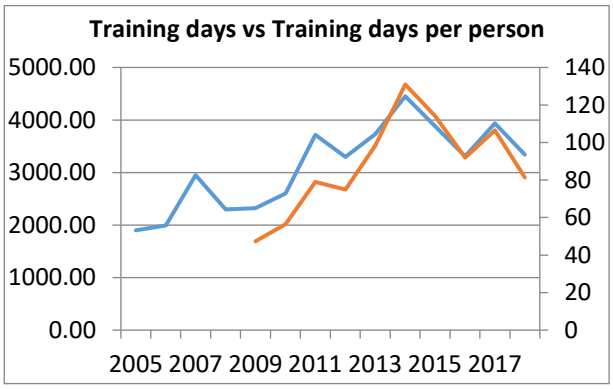
The citations metric shows an impressive upward trend, roughly doubling in the last five years to reach an average of roughly 65 citations per staff member. This is clear evidence of the success of the software supported by the programme. The considerable increase in the training days in recent years, as shown in the training days metric, is a significant contributing factor to the increased usage of the codes, as well as an additional indicator of the increase in the codes' user base. As our user base expands, more resource needs to be invested not just in the training but also in the user support.

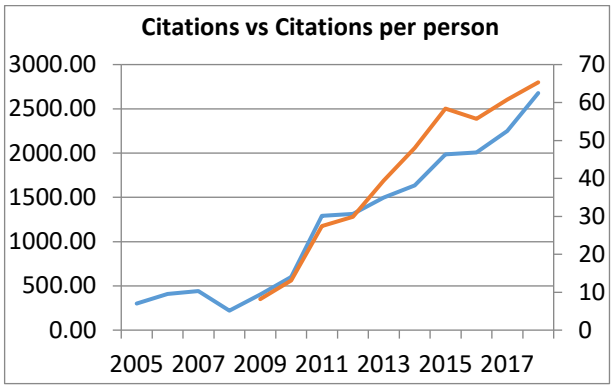
The yearly total numbers of publications since 2013 have been significantly lower than the yearly totals in the previous 8 years. This has been discussed before and correlates with a decrease in the funding level (from about 30 FTEs up to 2010/11 to about 25 after that), the doubling in code citations and steep increase in training days, showing that the programme has evolved to reach and support more and bigger communities. The recent downward trend in publications has been reversed this year, when 40 papers were published, versus the 27 published in 2016/17, a staggering ~50% increase. This is due to 10 out of the 13 projects publishing more than in the previous year. This may be due to some of the more recent projects reaching maturity, and to a decrease in training days compared to last year.

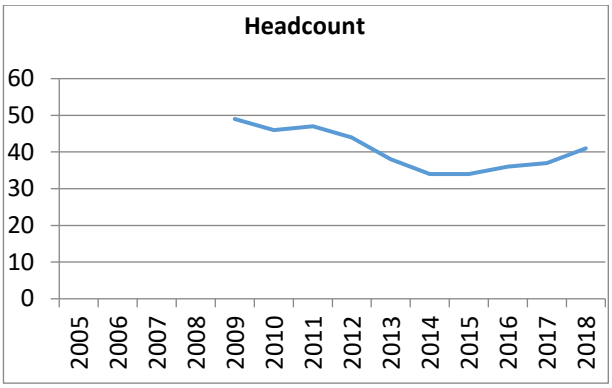
The presentations metric per person shows fluctuations around a roughly constant value. The headcount shows fluctuations around an average of 40.











Metrics breakdown by area

	FTE	Publications	Presentations	Training Days	Citations
CCP5 (including DL_ codes)	3.20	7.00	34.82	2255.50	460.00
CCP9	2.40	4.00	2.00	150.00	35.00
CCPmag	0.74	1.00	1.00	0.00	0.00
CCP-NC	1.30	6.00	7.00	212.00	474.00
CCPQ	1.86	2.00	7.00	30.50	100.00
CCP Plasma/HEC Plasma	0.95	1.00	4.00	13.00	104.00
CCPi	1.20	0.00	4.00	18.00	0.00
CCPPetMR	1.20	2.00	8.00	0.00	0.00
CCP-BioSim/HEC BioSim	2.20	3.00	1.34	27.00	7.00
MCC (including ChemShell, CRYSTAL)	2.50	5.50	18.83	453.50	475.00

UKCP (including CASTEP)	1.00	2.00	4.00	154.00	1233.00
UK-COMES	1.00	3.50	3.68	80.00	0.00
Software Outlook	2.00	3.00	2.00	0.00	0.00
Totals		**40.00**	**97.67**	**3393.50**	**2888.00**

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

Appendix 1: Detailed 2018 / 19 Plans

Project Office	Milestone	Target Date
	Attend CCP and HEC committee meetings as required	Ongoing
	Support CCP and HEC conferences and workshops as required	Ongoing
	Preparations for the SLA International Review 2018	Ongoing
	Carry out outreach activities (social media, brochures, talks)	Ongoing
	Maintain and update CoSeC web site	Ongoing
	Regular meetings with Technopolis to discuss progress with impact report	Ongoing
	Weekly internal STFC meeting to discuss progress with all CoSeC activities	Ongoing
	Liaise with Technopolis to launch impact report customer satisfaction survey	Q2 2018
	Arrange first payment to Technopolis	Q2 2018
	Arrange internal project meetings with funded CCPs and HECs – April 2017 – individual meetings	Q2 2018
	Prepare and submit annual CoSeC SLA report – June 2018	Q2 2018
	Arrange and attend the CCP Steering Panel June meeting	Q2 2018
	Attend the CoSeC SLA Steering Committee July meeting	Q2 2018
	Create new CCP web site – www.ccp.ac.uk	Q2 2018
	Assist Technopolis with impact report interviews	Q2 2018
	Complete one case study for each CoSeC funded project	Q3 2018
	Work with Technopolis to complete CoSeC impact report	Q3 2018
	Arrange internal project meetings with funded CCPs and HECs – July 2017 – DL / RAL site meetings	Q3 2018
	Compile and submit ARCHER renewal proposal	Q3 2018
	Prepare and submit interim CoSeC SLA report – December 2018	Q4 2018
	Prepare report / presentations / interviews and organise events for CoSeC international mid-term review	Q4 2018
	Arrange internal project meetings with funded CCPs and HECs – October 2017 – individual meetings	Q4 2018
	Arrange and attend the CCP Steering Panel December meeting	Q4 2018
	Attend the CoSeC SLA Steering Committee December meeting	Q4 2018
	Arrange CoSeC staff meeting	Q1 2019
	Arrange internal project meetings with funded CCPs and HECs – January 2019 – DL / RAL site meetings	Q1 2019

CCP5	Milestone	Target Date
Training & Outreach	Practical Exercises and Lecture Notes for CCP5 Summer school	Q2 2018
	Nuclear Materials Modelling Meeting	Q2 2018
	Preparation for Summer School	Q2 2018
	Introduction to programming for CCP5SS	Q2 2018
	Summer school and AGM, Midterm review	Q3 2018
	Outreach to Experimentalist and Industrialists	Q4 2018
	DL_Software training workshop	Q3 2018
	DL_Software training workshop	Q1 2019

ChemShell	Release of Py-ChemShell 2018	Q2 2018
	Development of new DL_SOFTWARE training materials for Py-ChemShell	Q3 2018
	Py-ChemShell plugin for Aten GUI	Q1 2019
DL_MESO	Release of DL_MESO version 2.7	Q2 2018
	Implementation of PPPM electrostatics in DL_MESO	Q3 2018
	Advanced mesoscale course at CCP5 Summer School	Q3 2018
	Implementation of fixed-length constraints	Q4 2018
DL_POLY	Refactoring work stage 1	Q2 2018
	Refactoring work stage 2	Q3 2018
	Two states EVB alpha release	Q4 2018
	EVB proof of concept application	Q1 2019
	Generalised GB alpha release	Q2 2018
	Generalised GB beta release	Q4 2018
DL_MONTE	Library of user cases extension	Q4 2018
	Extensive testing to full release	Q1 2019
DL_FIELD/DL_ANALYSER	Extension of xyz format recognition for the inorganic force fields.	Q3 2018
	Implement new features for characterisation of atomic interactions.	Q4 2018
	Maintenance and expansion of organic force field libraries	Q4 2018
	Release new DL_FIELD version 4.3 (testing + manual updates)	Q1 2019
	Release new DL_ANALYSER version 2.1 (testing+manual updates)	Q1 2019

CCP9	**Milestone**	**Target Date**
	Collaboration with Julie Staunton on permanent magnet materials, visit and discussion	ongoing
	Workshop: Questaal hands-on course	Q2 2018
	Workshop: Spin-Modelling workshop	Q2 2018
	Workshop on modelling nuclear materials	Q2 2018
	Submit EPSRC proposal with SuperSTEM/York/Leeds	Q2 2018
	~~Organize CCP9 working group/new chair~~ Organize CCP9 Young researcher's conference. Reorganize working group during Community meeting.	Q2 2018
	Implementation of SIC in LMF; development phase	Q2 2018
	Submit results on Ab initio magnetism of Mn3Sn (collaboration)	Q3 2018
	Results on TM-oxides	Q3 2018
	Publish article on magnetism in Gd-alloys	Q3 2018
	Organize widening participation workshop with SuperSTEM	Q3 2018
	Implementation of SIC in LMF; demonstration	Q3 2018
	Submit rare earth doped ceria article	Q4 2018
	Deliver capability to evaluate CF parameters in LMF (collaboration)	Q4 2018
	Workshop: KKR hands-on course (combined with CCPmag and SuperSTEM)	Q1 2019

CCP-mag	**Milestone**	**Target Date**
	Comparative study of exchange couplings	Q2 2018
	Co-ordinate session at IOP Magnetism 2018	Q2 2018

	Organize and run Spin Modelling workshop (co-funded by CECAM and Psi-k) in Lausanne	Q2 2018
	Co-ordinate SpinW course	Q2 2018
	Implementation of magnetic data in ESCDF library	Q3 2018
	Investigation of exchange couplings in non-collinear structures	Q3 2018
	First investigations into calculation of higher-order exchange couplings	Q4 2018
	Organize and run KKR course (possibly joint with CCP9)	Q1 2019
	Continued support for ISIS	ongoing

CCP-NC	Milestone	Target Date
	Improvement and dissemination of the Soprano Python library for crystallography	Ongoing
	Transitioning of the existing Magres database public interface from internal use to public use	Q4 2018
	Development of new methods for the treatment of nuclear quantum effects in NMR	Q4 2018
	Release of the Tran-Blaha and meta-GGAs functionals in CASTEP	Q4 2018
	Release with CASTEP of the NICS tool	Q4 2018
	Writing and submission of a paper on the topic of the Lorentz sphere and the range-dependent relationship between current fields and chemical shieldings in crystals	Q1 2019
	Integration of MagresView with NMR database	Q1 2019
	Pushing MagresView to version 2.0 – feasibility assessment of what it would take to release MagresView v2.0	Q1 2019
	Development of scripts and tools to encourage use of Soprano within the muon spectroscopy community	Q1 2019

CCPQ	Milestone	Target Date
Atomic R-matrix (+RMT)	MP: Continued test calculations of double continuum code as applied to RMT with regular feedback to QUB. Decision on which new systems to study and subsequent move to production work (using HEC Archer time if HEC is successful). Update objectives during year. Publish the code in the 50th anniversary issue of Computer Physics communications.	All year with mid-year update.
RMT	Possible projects (either for CCPQ support or possible eCSE-type applications): (i) AApply a 'flexible parallelization' scheme (as devised by AGS for the 2DRMP R-matrix code as part of the SERT project) to the post-laser-pulse system, reclaiming many MPI tasks previously devoted to inner region dipole calculations. (ii) RReduce inner region communication overhead: currently no consideration is given to how parallel blocks are split across nodes. Recalibrate task assignment to group smaller blocks together on a node and minimize the number of nodes used for larger blocks.	To be decided (decision Q2 2018) Q3 2018-Q1 2019

	Q2 2018: discussion of which project with QUB staff: (i) is currently preferred. AGS to perform this starting in ~Q3 following close of the SERT project and start of UK-AMOR work. Review in Q4.	
UKRMol+	AGS: Continued work on symmetry adaptation of atomic orbitals OR simultaneous diagonalization of several symmetries (as decided in Q1 meeting depending on preferences/expertise of the Flagship OU PDRA). Q2: complete TR after input from collaborators (Zdenek Masin, MBI Berlin) Q2 meeting: priority more likely to be given to the decided new project below (details to be confirmed). SEG/SESC's separate Flagship-funded Build Service support for UKRMol+ (and RMT) should be underway with the new (as of November 2017) staffing issues resolved (ongoing but effectively according to plan: TD's involvement to be decided in July)	Q2-Q3 2018 (to be confirmed)
UKRMol+	Possible projects (either for CCPQ support or possible eCSE-type applications): (1) RRelated to diagonalizers: find a practical workaround to limits the SLEPC library places on the number of eigenvalues that can be calculated due to memory allocation within SLEPC (either by efficient 'underpopulation' of nodes or by batched calculation of groups of eigenvalues via spectral transformations. (2) RRelated to diagonalizers: investigate when the large inner region Hamiltonian diagonalizer (MPI-SCATCI) should calculate all eigenvectors or use the 'partitioned R-matrix' method (Tennyson and colleagues) which concentrates on fewer roots at the expense of some additional linear algebra. Can this be automated while maintaining required accuracy (via an energy cutoff metric)? (3) Software development: integrate the diagonalization module MPI-SCATCI with the boundary module SWINTERF: these are currently run as two separate programs with associated write-to-disk of much intermediate data which can be held better in (distributed) memory. (4) IInvestigation of effective core potentials (for further discussion) Meeting in Q2 to decide on project. Work to take place Q2/Q3 – Q1 2019 with review in Q4 2018	To be decided Q2 2018 Q2/Q3 –Q1 2019
RMATREACT and PFARM	MP: resolve any final issues with the heavy-particle-collision version of PFARM, continue to expand range of potential interactions as required. COMPLETE subject to new requests for functionality (to be updated in the year) MP/AGS: Provide support for HEC software development work in which PFARM is combined with the resonance code package TIMEDELn (as needed, or more direct work if HEC is	Q2 2018 (with additional milestones to be selected and decided by Q2 2018)

	unsuccessful, to be agreed). UK-AMOR Q2 Strategy meeting decided this work would be done by AGS under UK-AMOR (HEC) core support with help from MP, with work to commence in Q3 and carry on to Q1 2019 with review in Q4 2018. The developed package will support time-delay and K-matrix resonance detection, and ideally look at complex poles of the S-matrix . MP/AGS: Maintain and keep up to date the novel technology (Xeon-Phi and GPU) versions of PFARM (all year): look for additional novel technology funding as appropriate. AGS will coordinate the new PRACE funding for further GPU optimization throughout the year. MP/AGS: Provide support for the PFARM/PSTGF performance comparisons contained in the HEC proposal (as needed, or more direct work if HEC is unsuccessful, to be agreed). Q2 meeting agreed that these tests will be performed by incorporating PSTGF into the PRACE accelerator benchmarking suite to supplement the limited CCPQ/HEC FTE funding.	Q3-Q1 2019 (actual work)
TNT and QUANTICS	Continued TNT work on I/O changes (from MATLAB to PYTHON) as/if required. Discussions on further support with ML. Milestones to be updated following CCPQ Steering Panel meeting. AK and ML have agreed a review/planning meeting to be held in June. Quantics work: continue performance optimization (if appropriate) and implement new project support as decided in Q1 (now Q2). [BOTH: the new (as of November 2017) staffing issues providing TNT and QUANTICS support should be resolved in time for 2018-2019: complete (Q2)]	Q2 2018 (also, additional milestones to be added in Q2 2018)
Antimatter	MP: agree milestones for more direct Aberdeen support. (Background additional antimatter work by MP as time allows through year)	Q2 2018 (additional milestones to be added in Q2 2018)
General	DJ (with MP if required) to support workshop admin for Attosecond (complete) and new workshops (as discussed in the CCPQ Steering Panel meeting). MP to maintain/expand publications page on CCPQ website and keep site up to date. Respond to new funding opportunities. Respond to new requests for CoSeC support from the diverse CCPQ community (with the approval of the Steering Panel). Continue to make sure that the support provide allows for interactions and (informal) training of PhD students and 'young' PDRAs. Q2-Q4 2018: SEG, MP to assist with transfer of CCPForge projects to GitHub (or other preferred) platforms: RMT and UKRmol have commenced this transfer already.	All year Q2-Q4 2018
CoSeC review	MP to coordinate and present CCPQ-support material for CoSeC international review.	Date to be confirmed (Q2 or Q3?)

CCPPlasma	Milestone	Target Date
	BOUT++: Optimize flagship physics modules, Hermes, Storm and GEMGF.	Q2 2018
	GS2: Identify the optimal set of modern data layouts needed in GS2 (that are both processor- and node-aware) to improve scalability for ambitious target problems. Design and implement the proposed layouts, optimizing communications using subcommunicators and shared memory.	Q3 2018
	BOUT++: Couple multigrid solver to implicit timestepping routines. Develop preconditioner to allow large time steps.	Q4 2018
	GS2: Assess impact of new data layouts on performance and scalability for target problems. Consider also optimization of communications for data not associated with distribution functions (e.g. the electromagnetic fields).	Q1 2019

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
	Working with CCPi Flagship team in improving Core Imaging Library (CIL) and integrating the codes from flagship into CIL.	Ongoing
	~~Setup a JIRA project management tool for Agile software development.~~	~~Q1 2018~~
	~~Optional: Optimise projection algorithms from community requests~~	~~Q1 2018~~
	~~Embed framework: Integrate the FISTA code in CIL into SAVU framework.~~	~~Q2 2018~~
	Add pre-processing stages beam hardening correction experiments; now to include publications.	~~Q1 2018~~ Q2 2018
	Embed CCPi software into DAaS virtual machine to allow users to perform analysis on their datasets from remote	Q2 2018
	Release updated version of Simpleflex segmentation algorithm developed together with Hamish Carr (Leeds) and his student. Distribute and collaborate with Diamond i12 staff to test the segmentation on real data.	Q2 2018
	2 summer students on Machine learning to explore available ML techniques for image processing and specifically on noise characterisation and correction.	Q3 2018
	Help to organise the main ToScA conference; September 2018	Q3 2018
	Embed framework: ISIS/IMAT– working with ULTRA and Phase 2 opens access up to users	Q3 2018
	Embed lab based framework: UoM/ UoS/ UoW	Q3 2018
	Collaboration: Working with Brian Bay (USA) on improving the digital volume correlation codes and distributing it to CCPi community.	Q4 2018
	Optional: Iterative code for the Nikon XTek X-Ray CT accelerated versions (Link/use tier 1 or tier 2 HPC)	Q4 2018
	Case Studies: Three case studies will be undertaken with ISIS/Diamond and Universities	~~Q3 2018~~ Q1 2019

CCPPET-MR	Milestone	Target Date
	Manage CCPPETMR website, mailing lists and data archives for both simulated and acquired data.	Ongoing
	Organise exec committee, working group meetings, developers' days and other events.	Ongoing
	Support current training courses.	Ongoing
	Assist in new proposal writing.	Ongoing
	Visit sites in the network to gain experience with a few selected packages for image reconstruction and to get others started with SIRF	Ongoing
	Set up and run continuous build and test system.	Ongoing
	Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide.	Ongoing
	Optional: Profiling (and possibly speed-up) of PET reconstruction.	Ongoing
	Write SIRF installation script for Windows, possibly using pre-compiled libraries.	Q2 2018
	Implement image data transformations between PET and MR and between different voxel grids and encapsulate image data into common SIRF image object.	Q2 2018
	Geometric information encoded in Image objects (co-registered PET and MR). Re-interpolating to a different grid size, transforming using rigid transformations.	Q2 2018
	Common Image objects for PET and MR. Therefore the Shape classes will work for both PET and MR.	Q2 2018
	Implement PET reconstruction with MR anatomical priors.	Q2 2018
	Full support for measured data (Siemens, GE non-TOF). MR only if ISMRMRD converter available. PET TOF support (no scatter).	~~Q2 2018~~ Q3 2018
	Implement iterative MR reconstruction with Gadgetron.	~~Q2 2018~~ Q3 2018
	SIRF Release 2.0	~~Q2 2018~~ Q4 2018
	Interface to motion estimation software.	~~Q3 2018~~ Q4 2018
	Motion-guided reconstruction. Spatial only at first, time sync later.	~~Q3 2018~~ Q1 2019
	MR reconstruction with PET prior.	~~Q4 2018~~ Q1 2019
	Joint PET-MR reconstruction using MATLAB or Python tools/toolboxes.	~~Q4 2018~~ Q1 2019
	Implementation of a few generic optimisation algorithms.	~~Q4 2018~~ Q1 2019
	List mode reconstruction without conversion to sinograms.	Q1 2019
	Joint motion estimation.	Q1 2019

CCPBioSim	Milestone	Target Date
	Lead organisation of the 3rd CCPBioSim/CCP5 Multiscale Modelling Conference	Q2 2018

	Complete testing and refinement of CCPBioSim website tutorials and integrate training workshop material into website.	Q2 2018
	~~Integration of FESetup with Longbow~~	~~Q3 2018~~
	Development of a benchmark set for relative alchemical free energy calculations to support integration of FESetup into BioSimSpace	Q3 2018
	Hold ChemShell training workshop for biomolecular QM/MM modelling in St.Andrews	Q4 2018
	Fix open technical issues, complete code review and improve robustness of FESetup to support integration of the code into BioSimSpace	Q4 2018
	Revision and online curation of membrane-bound protein multiscale modelling scripts from the first CCPBioSim software flagship project	Q4 2018
	Benchmarking of Cytochrome P450 model (CYP3A4) calculations on ARCHER	~~Q4 2018~~ Q1 2019
	~~Preliminary testing of BioSimSpace~~ Develop outline plan for BioSimSpace metadynamics node for binding kinetics calculations based on GROMACS/Plumed	Q1 2019

MCC	Milestone	Target Quarter
CRYSTAL	Test CRYSTAL INS spectra calculations on molecular crystals using the CRYSTAL/Mantid interface developed in 2016-2017. Documentation of the results. Potentially a paper to be submitted for publication.	Q2 2018
	Test DIIS solver in CRYSTAL17 on SCARF or Archer	Q2 2018
	Test D3 van der Waals corrections in CRYSTAL17	Q2 2018
	Start a collaboration with N Martsinovich and P Gillespie (University of Sheffield) concerning the simulation of excited states of grapheme-oxide systems with CRYSTAL. Discussion and set up of systems to study.	Q2 2018
	Improvement of sorting routines for excited states in the TD-DFT CRYSTAL module.	Q3 2018
	Coding the calculation of 2-electron response exchange integrals for TD-HF and TD-DFT. In collaboration with the University of Turin. This is an important development for the extension of TD-DFT in CRYSTAL. Visits to Turin University (1-2 weeks) possibly during Q2 2018 and Q4 2018 to discuss results and plan developments.	Q4 2018
	Fixing some issues with the parallel (Pcrystal) version of the TD-DFT module in the interface routines with the CP-HF code.	Q1 2019
	Deliver 4 lectures and 3 one-afternoon tutorials on CRYSTAL at the CCP5 Summer School on Molecular Simulation in Lancaster	Q3 2018
	Organisation of the MSSC2018 CRYSTAL Summer School at Imperial College London. Deliver 5 lectures and 5 one-afternoon tutorials on CRYSTAL usage.	Q3 2018
	Organise/attend monthly meetings of UK CRYSTAL developer at RAL, Oxford or Imperial College.	Q2 2018 – Q1 2019
	Submit revised version of a manuscript on excited state of combretastatin molecules. In collaboration with STFC Central Laser Facility.	Q2 2018

	Submit a revised version of a manuscript on the chemical reactivity of Ru-based catalysts, in collaboration with the ISIS Neutron and Muon source. This work is based on calculations carried out with CP2K.	Q2 2018
	Preparation of a review paper on excited state modelling radiation damage in X-ray macromolecular crystallography. In collaboration with the Diamond Light source. This work is based on calculations and modelling carried out with CRYSTAL and CPMD.	Q3 2018
	Supervision of Dr N Holzmann concerning two projects with CLF and ISIS.	Q2 2018 – Q1 2019
	Assistance with the preparation of a manuscript on excited state surfaces of combretastatin molecules using TD-DFT. (N Holzmann *et al.*). In collaboration with CLF.	Q1 2019
	Extend hybrid parallelism to 1 electron integrals and possibly to forces. Write documentation and disseminate with a publication.	Q1 2019
	Organise a Workshop on Electronic Structure Codes for Extended Systems in collaboratiion with UKCP.	Q1 2019
ChemShell / DL-FIND	Supervision of ChemShell work package in MCC “SAINT” software flagship project	Ongoing
	~~Implementation of freeze and thaw frozen density fragment optimisation in Python-ChemShell~~ Improve usability of nudged elastic band method in DL-FIND through improved initial path guesses, optimisation diagnostics and additional tutorials	Q3 2018
	Development of a Py-ChemShell interface to the ORCA QM code for embedded cluster calculations	~~Q1 2019~~ Q2 2018
	Support for ~~Tcl-ChemShell~~, Py-ChemShell ~~and GAMESS-UK~~ on ARCHER and Tier 2 systems (e.g. Thomas) including development of a directly-linked interface to DFTB+ for HPC work	~~Ongoing~~ Q1 2019
DL_POLY	Refactoring work, supervision and reporting	Ongoing
	Lectures for Summer School and DL_Software training	Q3 2018 and Q1 2019
	Collaborative Support	Ongoing
DL_FIELD	Run and manage large-scale graphene-cellulose nanocomposite simulations.	Q2 2018
	Automatic introduction or removal of core-shell models.	Q3 2018
	Automation of setting up mixed organic/inorganic parameters with different mixing schemes.	Q4 2018

UKCP	Milestone	Target Date
	Continued consolidation of Raman and NLO code, including user tutorial material.	Q2 2018
	Continued development of Jenkins CI platform to include build/test environments for Archer and Thomas.	Q2 2018
	Co-organization and teaching of CASTEP workshop in Oxford.	Q3 2018
	Bring electronic licensing system for academic CASTEP into production.	~~Q2 2018~~ Q3 2018
	Release management of CASTEP v19.1 including documentation and liaison with major HPC services.	Q4 2018
	Replace legacy "dispersion.pl" tool with a Python implementation.	Q4 2018

	Organisation of 2019 CASTEP "codefest" core developer workshop.	Q4 2018
	Prepare and release existing Genetic Algorithm CASTEP tool, including portability and application case study.	Q4 2018
	Extension of Raman/NLO code for phonon lifetimes to be applied in Bolzmann Transport Equations.	Q1 2019
	Implement van der Waals DFT (Dion) functional in CASTEP.	Q1 2019
	Release of the Tran-Blaha and meta-GGAs functionals in CASTEP	Q1 2019

UK-COMES	Milestone	Target Date
	Immersed boundary methods in DL_MESO	Q2 2018
	Body force implementation for shallow water equations in MPLB code	Q3 2018
	High density contrast Lishchuk algorithm for multiple fluid systems	Q4 2018
	Implement 3D MPLB code and test using Taylor-Green vortex	Q1 2019

HECBioSim	Milestone	Target Date
	Website maintenance tasks	Ongoing
	~~Establish the Training section of the website~~ Support Charlie Laughton with cloud based deployment of TioS	Q2 2018
	Longbow version 1.5.1	Q2 2018
	Jupyter demonstration project (Longbow/ChemShell)	Q3 2018
	Integration of FFEA and CCP-EM	Q4 2018
	Jupyter metadata project	Q1 2019

UK-AMOR	Milestone	Target Date
	Martin Plummer, Andrew Sunderland and Catherine Jones to attend Initial UK-AMOR management committee meeting at UCL and agree on initial support plans. [further milestones to be added following 2nd meeting (provisionally September, date to be confirmed)]	Q2 2018
	Andrew Sunderland to commence incorporation of PFARM into the TIMEDEL resonance package multi-level parallel framework and investigate 'plug-in' feasibility for existing UKRMol modules RESON and 'S-matrix' (alternatives to the time-delay method'. AGS to meet the new UCL PDRA when appointed and maintain contact.	Q3-Q4 2018
	Martin Plummer and Andrew Sunderland to investigate any opportunities for relative benchmarking of PFARM and complementary UK-AMOR code PSTGF (mainly used in electron ion collisions with a (simple) dominant known term in the interaction potential), using PRACE funding if possible.	Q2-Q4 2018
	Review of progress on resonance package work, new milestones for Andrew Sunderland for 2019-2020 agreed	Q1 2019

UKTC	Milestone	Target Date

	Investigate Lagrangian particle transport at scale using Code_Saturne.	Q2 2019

UKCTRF	Milestone	Target Date
	Assessing the status of the HAMISH development on ARCHER.	Q2 2019

Software Outlook	Milestone	Target Date
~~BOUT++ bottlenecks~~	~~Profile code to identify algorithmic bottlenecks~~	~~Q2 2018~~
~~BOUT++ preconditioners~~	~~Identify and implement new preconditioners to improve the convergence of the underlying iterative solvers~~	~~Q1 2019~~
~~CCP-WSI~~	~~Analyse new complex coupled systems and develop scalable coupling methods~~	~~Q1 2019~~
Hybrid programming	Initial framework identification survey and identify kernels from codes for comparative study	Q2 2018
Hybrid programming	Comparative study for the frameworks considered	Q1 2019
Physics/Maths Libraries	FFT: identify candidate codes and provide their attributes on website	Q2 2018
Physics/Maths Libraries	FFT: comparative study	Q4 2018
Physics/Maths Libraries	Linear Solvers: identify libraries and their attributes. Provide information on website	Q2 2018
Physics/Maths Libraries	Linear Solvers: survey appropriate solvers for use in EPOC, BOUT++ and other applicable codes	Q1 2019
General consultancy for CCPs	As required	Q1 2019

Appendix 2: Highlight Papers

CCP5

Shadi Fatayer, Bruno Schuler, Wolfram Steurer, Ivan Scivetti, Jascha Repp, Leo Gross, Mats Persson, and Gerhard Meyer. Reorganization energy upon charging a single molecule on an insulator measured by atomic force microscopy. Nature Nanotechnology (2018) DOI: 10.1038/s41565-018-0087-1

Structure and hydrogen bonding at the limits of liquid water stability - Flaviu Cipcigan, Vlad Sokhan, Glenn Martyna & Jason Crain, Scientific Reports volume 8, Article number: 1718(2018) doi:10.1038/s41598-017-18975-7

CCP9

Rare-earth/transition-metal magnetic interactions in pristine and (Ni,Fe)-doped YCo5 and GdCo5, Phys. Rev. Mat. 1, 02411 (2017), Christopher E. Patrick, Santosh Kumar, Geetha Balakrishnan, Rachel S. Edwards, Martin R. Lees, Eduardo Mendive-Tapia, Leon Petit, and Julie B. Staunton.

Calculating the Magnetic Anisotropy of Rare-Earth–Transition-Metal Ferrimagnets, Phys. Rev. Lett. 120, 097202 (2018), Christopher E. Patrick, Santosh Kumar, Geetha Balakrishnan, Rachel S. Edwards, Martin R. Lees, Leon Petit, and Julie B. Staunton.

CCPmag

Towards efficient data exchange and sharing for big-data driven materials science: Metadata and data formats, Luca Ghiringhelli, Christian Carbogno, Sergey Levchenko, Fawzi Mohamed, Georg Huhs, Martin Lüders, Micael Oliveira, and Matthias Scheffler. Accepted in npj Computational Materials

CCP-NC

Ab initio random structure searching of organic molecular solids: assessment and validation against experimental data, Miri Zilka, Dmytro V. Dudenko, Colan E. Hughes, P. Andrew Williams, Simone Sturniolo, W. Trent Franks, Chris J. Pickard, Jonathan R. Yates, Kenneth D. M. Harris and Steven P. Brown, Phys. Chem. Chem. Phys 38 (2017)

Machine learning unifies the modeling of materials and molecules - Albert P. Bartók, Sandip De, Carl Poelking, Noam Bernstein, James R. Kermode, Gábor Csányi and Michele Ceriotti, Science Advances, 3, e1701816 (2017)

CCPQ

S. Al-Assam, S.R. Clark and D. Jaksch, The tensor network theory library, J. Stat. Mech.093102 (2017).

J. Tennyson and S.N. Yurchenko, The ExoMol project: Software for computing large molecular line lists, Intern. J. Quantum Chem, 117, 92-103, (2017).

CCPBioSim

G.D.R. Matos, D.Y. Kyu, H.H. Loeffler, J.D. Chodera, M.R. Shirts and D.L. Mobley, “Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database”, J. Chem. Eng. Data, 62, 1559 (2017).

MCC

“Molecular dynamics study of CO2 absorption and desorption in zinc imidazolate frameworks” Min Gao, Alston J. Misquitta, Chenxing Yang, Ilian T. Todorov, Andreas Mutter¶c and Martin T. Dove, Molecular Systems Design & Engineering (The Royal Society of Chemistry), DOI: 10.1039/c7me00034k

Active site protein dynamics and solvent accessibility in copper nitrite reductase. K. Sen, S. Horrell, D. Kekilli, C.W. Yong, T.W. Keal, H. Atakisi, D.W. Moreau, R.E. Thorne, M.A. Hough and R.W. Strange, IUCrJ, 2017, 4, 495.

Leonardo Bernasconi, Andranik Kazaryan, Paola Belanzoni and Evert Jan Baerends, Catalytic Oxidation of Water with High-Spin Iron(IV)−Oxo Species: Role of the Water Solvent, ACS Catal. 2017, 7, 4018−4025

Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM
Z. Xie, Y. Sui, J. Buckeridge, C.R.A. Catlow, T.W. Keal, P. Sherwood, A. Walsh, D.O. Scanlon, S.M. Woodley and A. A. Sokol, Phys. Status Solidi A, 2017, 214, 1600445.

UK-COMES

Meng, J, Gu, X-J and Emerson, DR. Analysis of non-physical slip velocity in lattice Boltzmann simulations using the bounce-back scheme. Accepted by Journal of Computational Science and published online. https://doi.org/10.1016/j.jocs.2017.10.008

Anderson, RL, Bray, DL, Del Regno, A, Seaton, MA, Ferrante, AS and Warren, PB. Micelle formation in alkyl sulfate surfactants using dissipative particle dynamics. Accepted by Journal of Chemical Theory and Computation and published online. https://pubs.acs.org/doi/full/10.1021/acs.jctc.8b00075

Software Outlook

Using Mixed Precision within DL_POLY's Force and Energy Evaluations: Short-Range Two-Body Interactions, H. Sue Thorne, RAL Tech Report (Number TBC)

Using Mixed Precision within DL_POLY's Force and Energy Evaluations: Long-Range Interactions, H. Sue Thorne, RAL Tech Report (Number TBC)

Appendix 3: Major Code Developments

Code	Highlight	Comments
CCP5		
DL_POLY	• Extensive work on bringing up to date and including of Two Temperature Model developments, from 2012-2014 prototyping grant, took place. Verification and testing stages passed and code is at a mainstream version. Only manual clean up work and release remain as tasks.	• On-going, Q4 2017
	• Development and implementation of the SHAPE force field (generalised Gay-Berne) in DL_POLY:	• Complete
	• Integration of new data structures and parameters in the code.	• Complete for Serial version
	• Coding rigid body equation of motion for free biaxial shapes.	• Ongoing for Parallel
	• Developing equations for linked shapes forming a coarse-grained molecular representation, and coding them in DL_POLY. Tasks B) and C) initially for serial version and parallelising them using existing DL_POLY MPI strategy at a later stage.	• Ongoing
	• Development of Forward flux sampling into DL_POLY_4 together with eInfrastructure project	ongoing
	• Python utilities to prepare inputs and analyse outputs	ongoing
	• Gui to explore output of DL_POLY_4	ongoing
	• Development of Empirical Valance Bond (EVB) functionality:	• Complete
	• proof of concept via the implementation of a toy model to simulate the isomerization of a single malonaldehyde molecule.	• Complete
	• Implementation of EVB methodology	• Ongoing
	Consideration phase for DL_POLY_4 full reengineering to cope with the large amount low level changes required for a full scale parallel development.	Ongoing
DL_FIELD DL_ANALYSER	• Release DL_FIELD version 4.1.1 (April).	• Complete
	• Improvement of bio-inorganic systems: auto mixing of vdw parameters now possible for CLAYFF (clay mineral force fields).	• Complete
	• Introduction of VDW_FIX directive. Allows customised definition of the vdw interaction for a specific pair of atoms, including bio-inorganic systems.	• Complete

	• Inclusion of more Chemical Group detection for the DL_F Notation. Introduce DANAI, a standard notation for the description of atomistic interactions, including documentation. Carried out ethanoic acid simulation as a test case.	• Complete Complete
DL_MESO	• Wide-reaching changes were made to DL_MESO's DPD code to file reading and writing. In particular, writing of trajectory and restart state files has been extensively changed to use a data-gathering step among groups of processor cores and sequential writing from one core per group into single files. Reducing the number of files created improves usage of computers' file systems, as well as making it easier for users to manipulate and process those files. • A CUDA port of DL_MESO's DPD code for hosted NVIDIA GPUs is currently being carried out by Jony Castagna, while Silvia Chiacchiera has been developing software modules for E-CAM to calculate relevant properties for polarisable DPD models and check input and output file consistencies for DL_MESO calculations.	• Complete • E-CAM contributed work. Ongoing
DL_MONTE	• v.2.04 update release (end of October 2017): refactored the code for exclusion-lists to enable exclusion (or inclusion) of the VDW and electrostatic interactions between intra-molecular pairs: 1-2 (bonded), 1-3 (within angles), 1-4 (within dihedrals and inversion angles); clean-up and optimisation/refactoring of the Ewald summation (up to 20% speed-up) and the routines for nano-pore constraint, making the MFA long-range correction algorithm more stable in GCMC cases with the option of reading in previously obtained MFA data; addition of molecule orientational PSMC as opposed to configurational/translational algorithm.	• DL_MONTE flagship contributed work
ChemShell	• Released v3.7 in July, with new features including an extension of the task-farming parallelisation framework to support NWChem (Global Arrays). • Revised and updated interfaces to ORCA 4 and Dalton/LSDalton 2016. • Support for standalone execution of GULP, revised tutorial and compatibility with Tcl 8.6. • New Drupal-based website for chemshell.org and associated Twitter account @chemshproject.	• Complete • Complete • Compete • Complete

CCP9

Questaal	• Collective IO in HDF5 • New basis setup algorithm • Small bugfixes and enhancements for DFT and BSE infrastructure	• Working for the screened Coulomb interaction • Alternative basis strategy for highest accuracy calculations • Variety of miscellaneous bugfixes and usability improvements

CCPmag

ESCDF	New design of the library agreed and implemented.	Complete

CCP-NC

CASTEP	Tran-Blaha exchange potential	Beta testing
Soprano	• Simple NMR lineshape prediction • Computation of dipolar couplings in periodic systems • Bond order parameters • Generation of random interstitial defects with Poisson sphere distribution • Generation of substitutional defects (experimental) • Generation of additioned structures (experimental)	Deployed to the Python Package repository
Muon Outreach Application (name pending)	• Web app designed to provide an interactive experience reproducing some basic muon spectroscopy experiments Simulation of time-dependent signals for various field distributions and dynamical regimes	Prototype live on github.io
CASTEP	SCAN, TPSS meta-generalised gradient functionals	Ongoing
CASTEP	Primitive lattice finder interface	Ongoing

CCPQ

UKRMol(+)	Memory optimization of molecular orbital transformations,	On course with substantial gains (to be complete shortly after the reporting period). Further expansion of optimized code (new algorithm) agreed and carried out with substantial memory saving.
PFARM (accelerator version)	GPU and Xeon Phi architecture optimization	Complete (now to be part of the Unified European Application Suite for Accelerators).
PFARM (functionality)	Adaptation for 'heavy' collisions and extension of range outer region interaction potentials (new objective)	Proof of concept model potential work complete. Coding of 'heavy' reduced mass complete. Capability for a variety of interaction potentials added.
QUANTICS	Adapt manual build and test suite runs into the SESC Build Service (CI)	On course (to be complete shortly after the reporting period): Now

		effectively complete, waiting for feedback from GW

CCPPlasma / HECPlasma

BOUT++	• Release of BOUT++ v4.1.0 • Implementation of a new "SingleDataIterator" looping method.	• Full details announced on the BOUT++ website: https://boutproject.github.io//announcement/2017/09/22/v4.1.0_released.html • New looping method is between 1.5 and 5 times faster, depending on compiler and thread count. The method also vectorizes and OpenMP-parallelizes. Scheduled for inclusion in BOUT++ v4.2.0.
GS2	• Implementation of operator splitting to evolve collisions separately. • Implementation of "split domains" flexible data layout	• Speed up in initialization by factor of 1.6 to 4.4, depending on core count. Similar gains in time advance. Full details: http://gyrokinetics.sourceforge.net/wiki/index.php/Split_collisions • Parallelizing data more evenly with respect to different dimensions in the problem gives speed-up in time-advance of factor of 2.25 for test problem.

CCPi

CIL 0.9.3	• CIL is reorganised into two separate packages, which are shared library and application wrappers. Segmentation algorithm exposes new functionality: segmentation based on local and global isovalue, tree pruning based on new set of measures.New Avizo plugin. • New framework for the development of reconstruction algorithms (FISTA and FBPD in the first implementation) • Regularisation toolbox for reconstruction and image processing • Tomophantom, software for the creation of synthetic phantoms and projection data for CT reconstruction algorithm benchmarking.	• Complete • Complete • Complete • Complete
CIL – 0.9	• Release via conda channel • Parallel beam iterative reconstruction support • Cone beam iterative reconstruction support for XTek Lab based instrument. • FISTA regularizers based reconstruction • Missing Wedge reconstruction	• Complete • Complete • Complete • In progress • In progress
CCPi Segmentation	• Topology based segmentation • Case study on Diamond data	• Complete • In Progress

CCPPetMR

SIRF	• Create installation script (via CMake) that installs user-specified versions of SIRF and its pre-requisites on Linux and MacOS.	• Complete

	• Introduce post-build testing system based on CTest. • Implement PET acquisitions and images algebra. • Implement Matlab run-all-demos scripts and test scripts. • Implement storage scheme (file/memory) management for PET and MR acquisitions. • Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide. • Add more real data functionality (scattering etc.) • Add advanced features Appendix to User Guide • Provide initial support for reconstructing Siemens mMR PET data	• Complete • Complete • Complete • Complete • Ongoing • Ongoing • Complete • Complete
STIR	• Addition of Time-of-Flight capability • IO and processing for GE Signa PET/MR	• Ongoing • Ongoing

CCPBioSim

FESetup	Released version 1.2.1 with numerous bug fixes, general clean up and usability improvements	Complete
Code Review	Full code review of version 1.2.1 in preparation for integration into BioSimSpace project	Complete

MCC

ChemShell	• Cluster cutting module ported to Py-ChemShell • Interface to DFTB+ for fast semi-empirical DFT calculations • Release new version of Tcl-ChemShell (v3.7) on ARCHER	• Complete • Complete • Complete
DL_POLY	• RDF+errors • Thermal conductivity • Two temperature model integration	• Complete • In progress • Complete
DL_FIELD	• New inorganic features and reorganisation of inorganic FF libraries	• Complete
CRYSTAL	• Hybrid RPA/coupled-perturbed solver for excited states • Merge of UK and Italy versions of CRYSTAL17 for release	• Complete for pure DFT • Complete

UK-COMES

DL_MESO	• Membrane dynamics in two-dimensions to model fluid-filled vesicles • Extension of Lishchuk continuum-based fluid/fluid interactions to include density contrasts • Changes to output file writing to produce fewer files per timestep (by gathering data among groups of processor cores) • Implementation of immersed boundary method	• Complete • Complete (limited to two-dimensions: extension to three-dimensions to be done later) • Ongoing, to be extended to collaboratively write one file per timestep • Ongoing

MPLB (OPS-based LBE code)	• Testing of boundary conditions for pressure-driven flow and flow around a square • Preparation of documentation for application developers • Release of 2D code • Extension to three dimensions	• Complete • Complete • Imminent, subject to resolving licensing issues • Ongoing

HECBioSim

Longbow v1.5.0	• Relicensed from GPL to BSD. • Fixed user reported issue where on some machines the environment wasn't setup correctly. • Simplified the use of the API by dropping capitals and introducing simpler imports. • Recovery files are now autocleaned so reducing clutter. • Fixed a bad crash in the recovery mode. • Fixed bug that made cpu to spin up to 100% during job monitoring. • Fixed bug with examples downloads. • Fixed bug in setup script with python version checks. • Support for python 3.6 (tests etc).	All Complete

Appendix 4: Training and Outreach

CCP5

CCP5 training events cater for skill creation, problem solving and project assistance of the UK postgraduate (PG) students and young researchers. There are two main types of training events – the DL_Software training workshops, usually including an extra Hack Day, and the CCP5 Summer School to which we have already referred. The latter is also internationally focused and includes methodology lectures, case studies, demonstrations and own project work. The former caters predominantly for UK researchers and trains them in using the molecular modelling techniques and methodology embodied by the CCP5 software outputs – it is usually carried out in collaboration with other COSEC stewards from HEC-MCC, UKCOMES, leads from EPSRC projects EMCS, CCP5 flagship project, DL_MONTE, as well as an ISIS RSE lead. There is also a third mode: one-to-one training usually by short-term visits at Daresbury Laboratory by UK academics or by staff visits to collaborating institutions which also the main support mode of HEC-MCC.

- The DL_Software and Hack Day events organised at QMUL April 5-7, 2017 were attended by 25 participants. The event involved trainers from HEC-MCC, CCPBioSim and the flagship DL_MONTE project.
- Dr. Chin Yong gave an oral presentation: 'Introduction to molecular simulation' to Y12 students (15 pupils) at Altrincham Grammar School for Girls (April).
- The three days' splash introduction and training event on DL_MONTE at University of Bath (19-21 April) was a success. The event attracted 20 participants for UK and EU academia.
- Dr. Michael Seaton gave an overview of mesoscale capabilities within CCP5 at the CECAM/E-CAM workshop on state of the art in mesoscale and multiscale modelling (University College Dublin, May 2017). he also presented a talk on Poisson solvers in DL_MESO at the E-CAM Extended Software Development Workshop in Barcelona (July 2017).
- CCP5 had an invited presentation (on all software project) given by Chin Yong and 2 posters (Chin Yong and Andrey Brukhno) at the CCP-SAS meeting in Bristol, 25 June.
- CCP5 was represented by Andrey Brukhno with a presentation on scientific capability of CCP5 tools at the CCP-EM/CCP-BioSim meeting in Leeds, 14 July.
- Dr. Thomas Keal hosted one-on-one ChemShell training for Joe Jackson-Masters (University of Cardiff) on 18 July as part of a CCP5 summer project to develop new tutorials for Py-ChemShell.
- CCP5 Summer School was organised for the second year at University of Lancaster, in July 2017 for 10 days and was attended by 67 participants, from all over the world. Dr. Alin Elena took over from Dr. John Purton the running and organisational responsibilities for the school. The school involved not only distinguished academic speakers but also trainers and lecturers from other CoSeC consortia such as HEC-MCC, UKCOMES, UKCP and CCP5.
- Posters on DL_FIELD and DL_MONTE were presented at the workshop "Designing forcefields in an age of cheap computing", Sheffield, 26-28 July 2017.
- Posters on pharmaceutical studies and DL_Software application by workflows between DL_FIELD, DL_POLY and DL_ANALYSER were presented at ADDOPT biAnnual Meetings at Leeds (March) and Cambridge (October).
- Dr. Chin Yong gave a DL_Software presentation at an ADDoPT technical workshop at Leeds in July.
- CCP5 AGM conference organised at University of Strathclyde, 11-13 September, was attended by 87 participants, from UK and overseas, from academia and industry. The CoSeC team presented 5 posters on project work.
- A DL_Software and Hack Day event, 13-15 September, followed up after the AGM. The event attended 15 participants and involved trainers from HEC-MCC, CCPBioSim and the flagship DL_MONTE project.
- Prof. Mark Tuckerman from NYU concluded his UK tour as an international CCP5 visitor in May 2017.
- Dr. Kostya Tratchenko at QMUL, started using DL_POLY_4 for his master course in Molecular Simulations.

- Prof. Fernardo Escobedo, from Cornell University will be next year CCP5 international visitor, with visits at Cambridge University, Bath and more.
- Molecular Simulation research by Prof. Nora de Leeuw et al. using DL_POLY made the front cover September Issue of Journal of Molecular Chemistry B.

CCP9

Questaal hands-on workshop: A Questaal hands-on course was organized May 16-19 at Daresbury Laboratory. A primary focus of the hands-on workshop was on quasi-particle self-consistent GW (QSGW) theory and its applications. The course provided tutorials for both the theory of, and how to use, an all-electron code that implements both density functional theory and GW/quasi-particle self-consistent GW (QSGW) theory. The density-functional part is implemented with full potential generalization of the linearized muffin-tin orbitals (LMTO) theory, or LMTO+LAPW combined. Alltogether 30 students and 10 lecturers took part in the 4 day course. JJ gave a tutorial on the use of lmf.

CCP9 Young Researcher Event and Community Meeting: The event was held at Clare College, Cambridge, 10-11 April 2017, with altogether 95 participants. The programme included a keynote talk, presentations from recently appointed Academic Staff, updates on CCP9 Flagship Projects, and introductions to Research Software Engineering careers and the EPSRC Tier 2 Computer Centres. The Young Researchers presented their work in both pico-talks and posters. Q&A sessions were held to discuss career prospects, additional CCP9 YR activities, as well as CCP9 Strategy and future policy.

IMRC2017: LP presented the work on Gd-intermetallics at the International Materials Research Congress (invited), 20-25 August 2017

MSSC2017: BS was instructor at the CRYSTAL course “Ab-initio modelling in solid state chemistry” at Imperial College London in 18-22 September 2017

Nucler Power Institute of China visit: LP gave presentation on “Ab-initio modelling of fuel and reactor vessel materials”, at Daresbury Lab. 9 October 2017

CCP9 furthermore provided funding for:

- “Psi-k workshop on theory and simulation challenges of nano phase-change materials”, University of Warwick, 13-15 September 2017
- “ONETEP masterclass” University of Warwick, 29 August - 1 September 2017-10-26
- Widening participation workshop “Electronic structure of 2D materials: theory meets experiment” Diamond Light Source, 18-19 July 2017
- “17th European seminar on computational methods in quantum chemistry” Harper-Adams University, 11-14 July
- “Computational Physics and Materials Science: Total Energy and Force Methods 2018” Selwyn College, Cambridge, 9 – 11 January 2018
- “MSSC2017 – Ab initio Modelling in Sild State Chemistry”, Imperial College London, 18 – 22 September 2017

CCP9 funded a visit to Imperial College by Prof. Loredana Valenzano from the Department of Chemistry Michigan Technological University (USA). Two lectures were delivered at the Thomas Young Centre.

CCPmag

The “1st advanced Vampire workshop” was organised by Richard Evans (York) and held in York, September 10-15, 2017. This workshop was funded by CCP-mag.

CCP-NC

Simone Sturniolo has attended the 14th International Conference on Muon Spin Rotation, Relaxation and Resonance. Together with Leandro Liborio, funded by the ISIS muon group, they have presented the results of the joint CCP-NC/muon collaboration. Some of these results have also been submitted as a paper to the proceedings of the conference and has been published. They have also cooperated with the ISIS muon group to provide tutorials at their Muon spectroscopy school, introducing CCP-NC developed tools to the participants who had an interest in computational science.

In January, Simone Sturniolo gave a talk at the Oxford Institute of Physics titled “How to see atoms with a computer”. The objective was to present the work of CCP-NC, and the basic concepts of computational crystallography in general, to a wide non-expert audience.

Both Albert Bartok-Partay and Simone Sturniolo took part in the annual CASTEP workshop in August 2017 as tutors in the practical sessions. SS also contributed two practical lessons on use of CCP-NC supported software tools, while Albert created a document, now published on the new CCP-NC website that provides guidance on NMR-focused calculations, with suggestions on best practice.

CCPQ

Training activities provided by SLA/CoSeC for CCPQ members are generally in the form of specialized group meetings and one-to-one interactions (local and virtual): in this particular period (April to September) the support has concentrated on development more than training. However, various technical discussions and training/learning have taken place, including discussions on understanding the implementation of PFARM for ‘heavy particle’ collisions, training of the PRACE-funded staff on PFARM structure and targeted accelerator optimization along with provision of general benchmarking guidance for the optimized package, plus SESC guidance for QUANTICS on using the CI environment. MP’s planned technical discussions with Aberdeen (MM Law and a PhD student) on antihydrogen collisions have been deferred from this period by mutual agreement owing to availability and time-table clashes.

Since September, further discussions on double continuum codes took place around the Flagship meeting, MP and AGS met new OU PDRA Jakub Benda at Fortran 2013 course at DL and discussed UKRMol+. Theory discussions with UCL staff and students around ‘heavy particle’ R-matrix work have continued (for CCPQ and in advance of the new HEC). The general SESC guidance has continued.

CCPPlasma / HECPlasma

Joseph Parker provided nine days of GS2 training for PDRAs and new developers, and four days of BOUT++ training to a CCFE user and a new developer.

The new GS2 split collisions algorithm was documented on the GS2 wiki, and presented at the IoP Conference in November 2017.

CCPi

March 2018 Edoardo demoes the segmentation tool to Diamond i12 scientists (4 people).

On 12th November 2017 Sri gave a presentation on CIL at University of Manchester MXIF which was attended by 15 postdocs and researchers.

CCPi are co-sponsors of ToScA (6–8 September 2017): Tomography for Scientific Advancement symposium addressing wide range of applications based on tomography was attended by over 150 people. There were wide range of presentations from the speakers who are developing novel techniques in CT such as Laminography. There was one common theme that came up in the event was on digital volume correlation(DVC). CCPi team is planning to collaborate with Brian Bay in USA who is one of the pioneer in this field. CCPi team manned a stand as well as judged the best poster competition.

DLS (Diamond Light Source) Public open day (29 July 2017): CCPi demoed a VR application of tomography experiment instrument hall to nearly 200 members of public.

Dimensional XCT annual conference attended by Edoardo on 13 July 2017 and had discussions with the companies who are involved in tomography.

Organised a meeting with ICAL/Manchester Museum, Oxford museum and IMAT instrument scientist to discuss and then run testcases using neutron tomography for palaeontologists, 21 July 2017.

Imaging Data analysis at Diamond workshop was organised on 23 June 2017. Over 30 scientists attended it. Erica Yang gave a talk on the current CCPi software and future plans.

Advances in X-ray Imaging: Expanding the frontiers of Knowledge, this was attended by over 70 academics and CCPi core team was involved in organising the event. There was a pre-event fringe meeting with presentations and discussions on the future of Xray CT.

The network continues to promote training at other institutions as well as future software show and tell events through regular email newletters.

CCPPetMR

Our main outreach activities during the reported period continued to be our regular (every 6 weeks) Software Framework meetings, where we discussed our development progress with our potential users from PET-MR research community (KCL, Leeds, Manchester and other Universities' researchers) and representatives of major imaging scanner manufacturers, including Siemens and GE. We note that a majority of the universities and companies attending our developers' meetings are funded independently, i.e. outside of the core CCP support, indicating a strong community commitment. Furthermore, we have already attracted independently funded university researchers who are now actively contributing to the testing and documentation of the codes.

CCP PET-MR has funding to support the exchange of researchers (staff and students) between institutions. Two exchange programs were supported in the reported period: between UCL and Medical Imaging Research Center, Katholieke Universiteit Leuven (KUL), Leuven, Belgium, and between UCL and University of Leeds.

We contributed to the PET-MRI School for students and early stage researchers at PSMR 2017, the 6th Conference on PET-MRI and SPECT-MRI in May 2017, Lisbon, Portugal (25 attendants) with a hands-on PET-MR software training session using SIRF. We funded UK attendants to the school.

The 3rd UCL/UCLH PET MRI Course took place on 11-13 May 2017 and KCL Course on Simultaneous PET-MR: Science and Practice on 28 June 2017.

CCPBioSim

Tom Keal led the CCPBioSim training workshop "QM/MM modelling of biomolecular systems with ChemShell" at Daresbury Laboratory on 9 May, which was well attended with 16 people joining the course.

MCC

- Posters on pharmaceutical studies and DL_Software application by workflows between DL_FIELD, DL_POLY and DL_ANALYSER were presented at ADDOPT biAnnual Meetings at Leeds (March) and Cambridge (October).
- Dr. Ilian Todorov gave three lectures at the CCP5 Summer School at University of Lancaster, in July 2017. The 10 days' school was attended by 67 participants from all over the world. The school involved not only distinguished academic speakers but also trainers and lecturers from other CoSeC consortia such as HEC-MCC, UKCOMES, UKCP and CCP5.
- Dr. Chin Yong gave a DL_Software presentation at an ADDoPT technical workshop at Leeds in July.
- Posters on DL_FIELD and DL_MONTE were presented at the workshop "Designing forcefields in an age of cheap computing", Sheffield, 26-28 July 2017.

- Dr. Thomas Keal gave an invited talk on “QM/MM modelling of enzymes and heterogeneous catalysis” at the MGMS QM/MM Methods and Applications Conference held at the University of Manchester on 5 September.
- A DL_Software and Hack Day event, 13-15 September, followed up after the AGM. The event attended 15 participants and involved trainers from HEC-MCC, CCPBioSim and the flagship DL_MONTE project.
- Dr. Kostya Tratchenko at QMUL, started using DL_POLY_4 for his master course in Molecular Simulations.
- Molecular Simulation research by Prof. Nora de Leeuw et al. using DL_POLY made the front cover September Issue of Journal of Molecular Chemistry B.
- MSSC2017 CRYSTAL Summer School, Imperial College London (18-22 September 2017) – This 5-day workshop includes morning lectures and afternoon tutorials on CRYSTAL and targets specifically beginner users of CRYSTAL. 5 lectures and 5 one-afternoon tutorials delivered by STFC staff (LB, BS)
- CCP5 Summer School, University of Lancaster (9-18 July 2017) – We delivered 4 lectures and 3 one-afternoon tutorials on the CRYSTAL code, quantum chemistry, DFT and TD-DFT. 4 lectures and 3 one-afternoon tutorials delivered by STFC staff
- Informal support to CRYSTAL users: ca. 1 afternoon per week (ca. 20 days)
- Technical support to STFC SCARF cluster CRYSTAL users (CRYSTAL porting, testing, installation, scripting for users, etc.): ca. 1 day per week (ca. 50 days)
- Support for CRYSTAL for new users in the Department of Chemistry at the University of Almeria (Spain): ca. 10 days.
- Tom Keal gave an invited talk on “QM/MM modelling of enzymes and heterogeneous catalysis” at the MGMS QM/MM Methods and Applications Conference held at the University of Manchester on 5 September
- Tom Keal and You Lu visited the groups of David Willock and Andrew Logsdail at Cardiff University on 5 December. You Lu gave a seminar on Py-ChemShell developments. One-to-one training was given and future developments discussed with the groups.
- Tom Keal and You Lu hosted Alex Gheorgiu from Peter Coveney’s group at UCL for ChemShell training (14-15 February 2018)
- A DL_Software training course was held at Daresbury on 19-22 February, with MCC staff providing training in DL_POLY, DL_FIELD and ChemShell among other codes.

UKCP

Two Density Functional Theory “taster” sessions were held at the ISIS Neutron Training Course. The half-day activities expose ISIS users to key concepts of computational modelling and DFT in the context of CASTEP and vibrational spectroscopy.

One-to-one training with Rebecca Fair (STFC-SCD) working on an interface between CASTEP and HORACE for the analysis of magnetic excitations.

Outreach discussions with the ISIS Excitations Group, particularly Toby Perring, to advise on the software development project “PACE” – a multi-year project to produce an efficient suite of tools for the analysis of magnetic excitations. This is a ground-breaking project funded by ISIS in lieu of an instrument upgrade. Part of the outreach activity included the co-organization of a one day meeting between members of ISIS and SCD to establish key areas of expertise.

UK-COMES

Three DL_SOFTWARE training workshops took place: one at Queen Mary University of London in April 2017 (20 participants), one at the University of Strathclyde in September 2017 (10 participants) and one at Daresbury Laboratory in February 2018 (24 participants).

The UKCOMES technical meeting was held at Daresbury Laboratory on 21 June 2017, organised by Jianping Meng, Dave Emerson and Michael Seaton, and was attended by 30 UKCOMES consortium members as well as representatives of its Industrial Advisory Board (including representatives from Unilever, Airbus and Mitsubishi).

As part of a trip in November 2017 funded by The Royal Society for UK-China International Exchanges for STFC to establish new collaborations, Michael Seaton gave presentations on DL_MESO and its capabilities at the State Key Laboratory of Hydraulics (20 participants) and Mountain River Engineering, Sichuan University and the National Supercomputing Centre in Wuxi (25 participants).

HECBioSim

HECBioSim does not yet offer its own training programme with the training being delivered from CCPBioSim. However, HECBioSim has supported the development of the new CCPBioSim training platform. This platform consists of self-contained training courses that can be completed through a web interface (Jupyter) either individually or at a traditional training workshop or surgery. The intention is that this will form the basis of our community effort to increase the breadth and complexity of training subjects by providing a modular training programme that can be pulled together into structured courses or form prerequisites for more complex workshops. The structure of the workshops follow a particular style and is encouraged to host out of the CCPBioSim GitHub repository with any specialist software having the option of being provided through cloud infrastructure. This setup was trialled at the CCPBioSim training week 2018 (https://ccpbiosim.github.io/workshop/events/bristol2018/).

Software Outlook

Software Outlook is finalising their new training material, which will include webinars, slides, detailed handouts and worked examples to help CCP/HECs to make use of our recommendations. STFC's Hartree Centre are providing us with the infrastructure to do this. We are also working to restore our web presence following changes in the set-up of STFC's websites. At the end of this reporting period, we heard that we had been successful in our application for the softwareoutlook.ac.uk domain.

Appendix 5: Risks

The following table outlines the major risks identified over the current year.

Risk No	Description	Likeli-hood	Impact	Mitigation Strategy	Previous status	Current status	Risk Owner
1	Recruitment of staff with appropriate skills	Medium	High	Staff skills plan under development. Graduate recruitment and training programme.	Amber	Amber	Barbara Montanari
2	Loss of key staff	Medium	High	Expand programme to create new opportunities via portfolio review. Succession plan for senior staff. Recruit.	Red, due to recent loss of staff	Amber Currently Stable	Barbara Montanari
3	Staff Illness and absences	Medium	Medium	Staff are funded by STFC central funds when on sick. Adjust workload of other staff, and SLA funds to set up additional contracts	N/A	Amber Plans for current and recent issues are working well	Barbara Montanari
4	Access to systems for developme nt and novel architecture systems for evaluation and developme nt work.	Low	High	Investment in Energy Efficient Computing Research Programme	Green	Green	Barbara Montanari
5	Time overrun on objectives	Medium	Medium	Progress against key deliverables reviewed monthly alongside progress by collaborating groups. Tasks reprioritised to meet timelines.	Green	Amber	Barbara Montanari

6	Project overspend	Low	Medium	Quarterly outturns for programme with monthly checks to monitor financial status. Reschedule programme.	Green	Amber	Barbara Montanari
7	Quality/ Relevance/ Customer satisfaction/ Value for money	Low	High	Proactive programme of interaction with academic customers. Strong and regular interaction with Steering Group. Performance metrics and reviews.	Amber	Amber	EPSRC / Barbara Montanari
8	Software Quality To ensure reusable/ modular/ correct/ portable software	Medium	Medium	Establish programme of Software Engineering support through additional bid and actively involve internal and external computer scientists.	Green Plans being implemented in key software packages.	Green Activities now funded by five year grant.	Catherine Jones
9	Mismatch of current staff skills to new programme	Low	Medium	Once work plans are finalised recruitments may need to take place.	New	Green Projects fully staffed	Barbara Montanari

Likelihood: Low: Next Year Medium: Next 6 months High: Next quarter
Impact: Low: delay 3 months Medium: delay 6 months High: delay 12 months

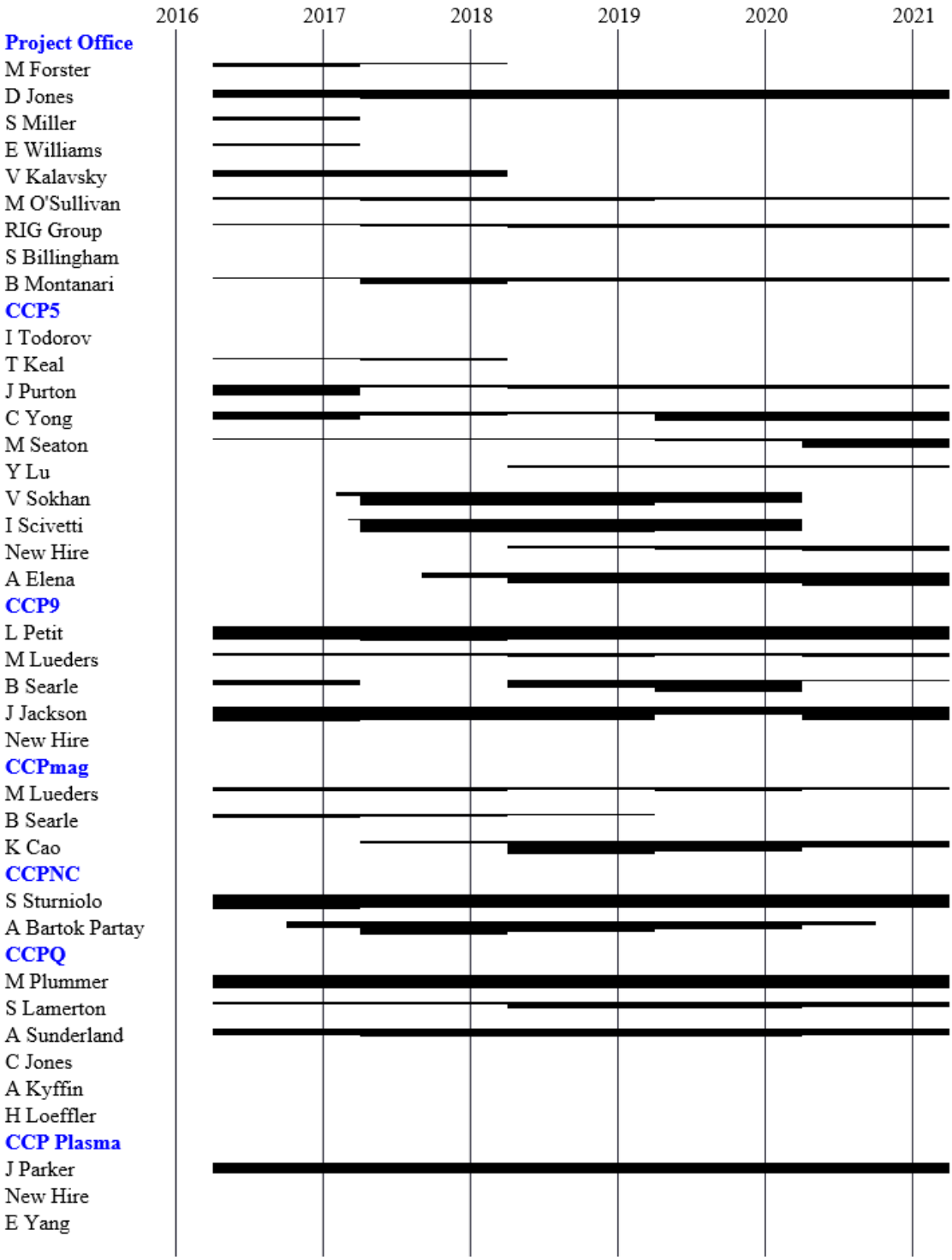
Appendix 6: Planned Staff to Project Bookings

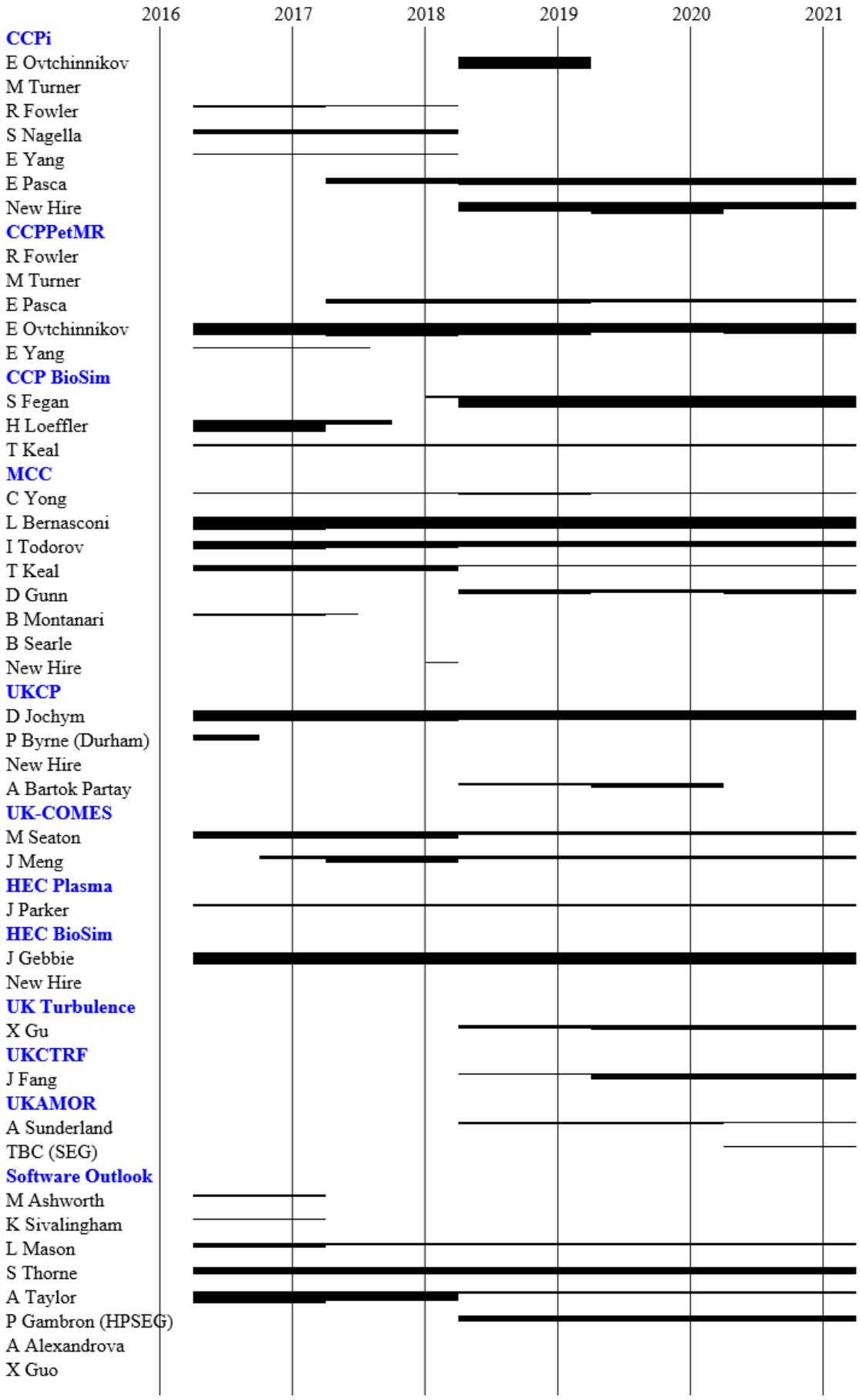
The following table shows the planned staff to project bookings for FY 2018/19.

Project Office		FTE	Project Total
	D Jones	0.70	
	M O'Sullivan	0.25	
	B Montanari	0.25	
	RIG Group	0.25	
			1.45
CCP5			
	J Purton	0.25	
	C Yong	0.20	
	M Seaton	0.07	
	Y Lu	0.20	
	V Sokhan	1.00	
	I Scivetti	1.00	
	A Elena	0.76	
	I Todorov	0.03	
	New Hire	0.17	
			3.68
CCP9			
	L Petit	1.00	
	M Lueders	0.26	
	J Jackson	1.00	
	B Searle	0.60	
	New Hire	0.04	
			2.90
CCPmag			
	M Lueders	0.22	
	B Searle	0.05	
	K Cao	0.96	
			1.23
CCPNC			
	S Sturniolo	1.00	
	A Bartok Partay	0.80	
			1.80
CCPQ			
	M Plummer	1.00	
	S Lamerton	0.45	
	A Sunderland	0.55	
			2.00
CCP Plasma			
	J Parker	0.80	
			0.80

CCPi			
	E Pasca	0.60	
	New Hire	0.75	
			1.35
CCPPetMR			
	E Pasca	0.40	
	E Ovtchinnikov	1.00	
			1.40
CCP BioSim			
	S Fegan	1.00	
	T Keal	0.20	
			1.20
MCC			
	C Yong	0.23	
	L Bernasconi	1.00	
	I Todorov	0.46	
	T Keal	0.10	
	D Gunn	0.36	
			2.15
UKCP			
	D Jochym	0.80	
	A Bartok Partay	0.20	
			1.00
UK-COMES			
	M Seaton	0.30	
	J Meng	0.30	
			0.60
HEC Plasma			
	J Parker	0.20	
			0.20
HEC BioSim			
	J Gebbie	1.00	
			1.00
UKTC			
	X Gu	0.30	
			0.30
UKCTRF			
	J Fang	0.13	
			0.13
UKAMOR			
	A Sunderland	0.20	
			0.20
Software Outlook			
	L Mason	0.20	

	S Thorne	0.60	
	A Taylor	0.20	
	P Gambron	0.50	
			1.50


2016
2017
2018
2019
2020
2021
Project Office
M Forster
D Jones
S Miller
E Williams
V Kalavsky
M O'Sullivan
RIG Group
S Billingham
B Montanari
CCP5
I Todorov
T Keal
J Purton
C Yong
M Seaton
Y Lu
V Sokhan
I Scivetti
New Hire
A Elena
CCP9
L Petit
M Lueders
B Searle
J Jackson
New Hire
CCPmag
M Lueders
B Searle
K Cao
CCPNC
S Sturniolo
A Bartok Partay
CCPQ
M Plummer
S Lamerton
A Sunderland
C Jones
A Kyffin
H Loeffler
CCP Plasma
J Parker
New Hire
E Yang


2016
2017
2018
2019
2020
2021
CCPi
E Ovtchinnikov
M Turner
R Fowler
S Nagella
E Yang
E Pasca
New Hire
CCPPetMR
R Fowler
M Turner
E Pasca
E Ovtchinnikov
E Yang
CCP BioSim
S Fegan
H Loeffler
T Keal
MCC
C Yong
L Bernasconi
I Todorov
T Keal
D Gunn
B Montanari
B Searle
New Hire
UKCP
D Jochym
P Byrne (Durham)
New Hire
A Bartok Partay
UK-COMES
M Seaton
J Meng
HEC Plasma
J Parker
HEC BioSim
J Gebbie
New Hire
UK Turbulence
X Gu
UKCTRF
J Fang
UKAMOR
A Sunderland
TBC (SEG)
Software Outlook
M Ashworth
K Sivalingham
L Mason
S Thorne
A Taylor
P Gambron (HPSEG)
A Alexandrova
X Guo

Appendix 7: Glossary

ARCHER	The UK's National Computing Service
BEIS	Department of Business, Energy and Industrial Strategy
BOUT++	A framework for writing fluid and plasma simulations in curvilinear geometry
BuildBot	An automated compilation system used for testing software.
CASTEP	A plane wave based total energy code for solid state and materials simulations.
CCP	Collaborative Computational Project. The Collaborative Computational Projects (CCPs) bring together leading UK expertise in key fields of computational research to tackle large-scale scientific software development, maintenance and distribution. Each project represents many years of intellectual and financial investment. The aim is to capitalise on this investment by encouraging widespread and long-term use of the software, and by fostering new initiatives such as High End Computing consortia.
CCP5	CCP on the computer simulation of condensed phases.
CCP9	CCP on computational electronic structure of condensed matter
CCPBioSim	CCP on biomolecular simulation at the life sciences interface
CCPForge	Software repository and distribution service
CCPi	CCP on tomographic imaging
CCPmag	CCP on computational magnetism
CCPNC	CCP on NMR crystallography
CCP PetMR	CCP on synergistic PET-MR reconstruction
CCP Plasma	The Plasma-CCP Network
CCPQ	CCP on quantum dynamics in atomic molecular and optical physics
ChemShell	A computational chemistry environment that supports standard quantum chemical or force field calculations. Its main strength lies in hybrid QM/MM calculations.
CIL	Core Imaging Library
CIUK	Computing Insight UK – an annual HPC Conference organised by STFC's Scientific Computing Department

CoSeC	the Computational Science Centre for Research Communities
CPU	Central processing unit
CRYSTAL	A local basis set first principles code for studies of 0, 1, 2 and 3 dimensional periodic systems
DAFNI	The Data & Analytics Facility for National Infrastructure project
DFPT	Density functional perturbation theory
DFT	Density functional theory
DIAMOND	The UK Synchrotron Radiation Source
DL	Daresbury Laboratory
DL_FIELD	Package to apply biological force fields to molecular simulations data
DL_FIND	A library of optimisation packages
DL_MESO	Mesoscopic modelling package
DL_MONTE	Monte Carlo simulations package
DL_POLY & DL_POLY4	A general purpose molecular dynamics package.
DLV	Daresbury Laboratory Visualize Package
DPD	Dissipative particle dynamics
EPSRC	Engineering and Physical Sciences Research Council
FESetup	A tool to automate the setup of alchemical free energy (AFE) simulations like thermodynamic integration (TI) and free energy perturbation (FEP)
FPGA	Field programmable gate array
FTE	Full time equivalent
GAMESS-UK	A first principles quantum chemistry package
GPGPU	General purpose graphical processing unit
GPU	Graphical processing unit
GS2	A physics application, developed to study low-frequency turbulence in magnetized plasma
HEC	High End Computing
HECBioSim	High-End Computing Consortium in biomolecular simulation

HEC Plasma	Plasma High-end Computing Consortium
HF	Hartree-Fock
HPC	High performance computing
HUTSEPOT	All electron band theory code
I/O	Input/Output
ISIS	Neutron spallation source located at the Rutherford Appleton Laboratory
JMOL	An open-source Java viewer for chemical structures in 3D
KKR	Korringa-Kohn-Rostoker
LBE	Lattice Boltzmann Equation
LMF	An LMTO code
LMTO	Linear muffin tin orbital
KS	Kohn-Sham
MAGMA	A mathematical library for GPGPUs
MagresView	Visualisation tool developed by CCPNC
Materials Chemistry Consortium	UK Materials Chemistry Consortium
MC	Monte Carlo
MD	Molecular dynamics
MP	Member of parliament
MPI	Message passing interface – a parallel programming paradigm in which involves the creation of multiple tasks.
NDA	Non-disclosure agreement
NMR	Nuclear magnetic resonance
NSF	National Science Foundation – American grant funding agency
NWCHEM	Quantum chemistry package from Pacific North West Laboratory
ONETEP	Order-N Electronic Total Energy Package
OPEN-MP	A method of programming parallel applications on shared memory systems in which applications are separated into multiple threads.
PB	Peta-bytes

PDRA	Post-doctoral research associate
PPPM	Particle-particle particle-mesh
PRACE	A European project looking at advantage computing architectures
PRMAT	A massively parallel R-Matrix code
QM/MM	Coupled quantum mechanical and molecular modelling simulations
Quantics	A package based on the MCTDH algorithm for molecular quantum dynamics
Questaal	A suite of electronic structure programs. The codes can be used to model arbitrary materials, but they are mostly designed to answer condensed-matter theory questions about solid state (periodic) structures.
RAL	Rutherford Appleton Laboratory
R-Matrix Suite	A set of programs for electron (positron) -atom and -molecule scattering, (ultrafast) laser pulse interactions and related problems
RSE	Research Software Engineer
ScaleMP	Software that allows the creation of virtual shared memory systems
SCD	Scientific Computing Department
SIRF	Synergistic Image Reconstruction Framework developed by CCPPetMR
SISC	Journal on Scientific Computing
SKA	Square kilometre array project
SLA	Service Level Agreement
STFC	Science and Technology Facilities Council
TD-DFT	Time dependant density functional theory
TNT	A package coding Tensor Network Theory for coherent many-body nuclear dynamics
ToScA	Tomography for Scientific Advancement Symposium
UK-AMOR	UK Atomic, Molecular and Optical physics R-matrix Consortium
UKCP	The United Kingdom Carr-Parrinello Consortium
UK-COMES	UK Consortium on Mesoscale Engineering Sciences

UKCTRF	UK Consortium on Turbulent Reacting Flows
UKCRIC	UK Collaboration for Research on Infrastructure and Cities
UKTC	United Kingdom Turbulence Comsortium
UKRI	UK Research and Innovation - the home of world class research and innovation in the UK