CoSeC

Computational Science Centre for Research Communities

EPSRC Service Level Agreement with STFC for Computational Science Support

FY 2016/17 Report and Update on FY 2017/18 Work Plans

June 2017

Table of Contents

Background

The Computational Science Centre for Research Communities (CoSeC) aims to enrich computational science and engineering research by enabling research communities to advance their work and exploit the full spectrum of local and national computing facilities. It ensures the continued development and long-term maintenance of software which makes optimum use of the whole range of hardware available to the scientific community, from the desktop to the most powerful national supercomputing facilities.

This document refers specifically to the CoSeC activities in the areas of interest to the UK Engineering and Physical Sciences Research Council (EPSRC). The EPSRC funds CoSec activities through a Service Level Agreement (SLA) with STFC, which delivers work undertaken by staff at its Daresbury and Rutherford Appleton Laboratories. This work has three main components:

- **Support for the EPSRC Collaborative Computational Projects (CCPs)** by developing, maintaining and providing expertise, software and training for a large suite of codes on a range of hardware platforms. These scientific and technical efforts are complemented by the coordination of networking events and knowledge exchange for the CCP communities; for example, organising workshops, conferences, newsletters, program libraries and visits from overseas scientists.
- **Support for the High-End Computing (HEC) consortia** organised in HEC consortia, funded by EPSRC, for distributing computer resources available at the UK national supercomputing service. This work focusses on the development of new scientific functionality in highly scalable parallel applications, often developing the high performance computing (HPC) algorithms required to make the codes developed under CCP programme suitable for deployment on the national facilities.
- **The Software Outlook** activity, which 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.

The main deliverables of the SLA programme fall into the following categories:

- Codes with new functionality, maintained and supported, that advance computational sciences but also support effective and efficient exploitation of the full spectrum of computing facilities supported by EPSRC.
- Evaluation of new hardware and software technologies.
- Researchers trained in HPC and computational science and engineering methods.
- Scientific and technical workshops.
- Co-ordination of computational science and engineering networking activities.
- Strategic support to the UK Academic Computational Science & Engineering Community.

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 Ilian Todorov
CCP9	Computational Electronic Structure of Condensed Matter	Prof Mike Payne	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 Martin Turner
CCP-PET/MR	Computational Collaborative Project in Synergistic PET-MR Reconstruction	Prof Kris Thielemans	Dr Martin Turner
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 Barbara Montanari
HEC-BioSim	High-End Computing Consortium in biomolecular simulation	Prof Adrian Mulholland	Dr Tom Keal
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

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
HEC-BioSim	1.0
UKCP	1.0
HEC Plasma	0.2
UK COMES	1.0

STFC News

Following Paul Sherwood's retirement in September 2016 Mark Forster joined STFC as Head of the Applications Division and Deputy Director of the Scientific Computing Department. Mark has now moved over to the Hartree Centre with Barbara Montanari appointed Acting Head of the Applications Division. Barbara is also managing the SLA activities in association with Damian Jones.

The SLA is being renamed as CoSeC "Computational Science Centre for Research Communities" and we expect this to be launched in the autumn. The aim of this rebranding is to raise the profile and visibility of the SLA activities.

From 1 November 2016 Brian Bowsher is STFC's new Chief Executive. He has been a member of Council since 2013 and also chaired its Finance Committee. Brian has led a number of major science activities in both the public and private sector. Most recently, he was the Managing Director of the National Physical Laboratory (NPL), the UK's National Measurement Institute, from 2009 to his retirement in 2015. NPL's science outputs and impact increased significantly during Brian's tenure; NPL also grew its third-party work by 11% pa to the point that it accounted for over 40% of the lab's revenue. From 2012 to 2016, Brian was a member of the **Comite international des poids et mesures (CIPM)**, the world-wide authority on measurement; he also chaired its Finance Committee. Brian continues to be a member of the International Advisory Board to the Chinese National Measurement Institute and has also recently been appointed as lead of the UKRI Infrastructure Group.

Following on from the publication of the STFC computing review, Tony Hey, (STFC's Chief Data Scientist) has been leading a working group to develop the STFC e-infrastructure strategy, which is built on the STFC Strategic Computing Review (published in December 2015) and is now close to finalisation. The strategy is being presented to science board in June, and will then go to Executive board later in the year.

CoSeC Project Office

The Project Office was established in April 2015 with the remit to provide support to the SLA funded CCPs and HEC Consortia and complete the SLA reporting required by EPSRC and the Steering Committee. A portion equal to 0.95 FTEs of the resource for the Project Office is provided by the CCP communities (i.e., 7% of their granted support).

Collection and collation of data for the mid-term and annual SLA reports is a major role for the project office. A number of new processes have been put in place to streamline this process, including the introduction of reporting templates and the use of SharePoint as a repository. The recurring issue of problems with CCP web sites has also been addressed and a move towards Drupal software was initiated, with most projects now migrated onto the Drupal platform. Ongoing support for the Drupal web sites is provided through the Project Office by the RIG group at Rutherford Appleton Laboratory.

The Project Office remit has now been expanded further to include monitoring of effort bookings and spend, monitoring of progress against project job plans and milestones, support for funded CCP and HEC conferences and workshops, monitoring of the SLA allocation on ARCHER, and advice to increase the impact and dissemination of the work completed using SLA funding through the Impact Manager Marion O'Sullivan.

Project Office – Summary Report (1 April 2016 – 31 March 2017)

An important activity for the project office over the last reporting period has been the continuation of quarterly project meetings with the STFC based co-ordinators of each of the SLA funded CCPs and HECs. These meetings allow the project office to track the progress of job plans for each of the projects but also importantly allow communication between the projects and the support staff to ensure that any issues that require attention are addressed and areas where support can be offered are identified. The meetings are proving very beneficial to both the staff funded by the SLA and the project office.

Work is continuing on the migration of project websites to new Drupal based web sites where required. For example, CCP5 and CCP9 recently went live with their Drupal site following the successful transfer of information from their previous static HTML site. With the help of the support staff at Rutherford Appleton Laboratory we are now also in a position where we can create accounts on the Drupal sites for people external to STFC, which in turn allows them to edit the sites. Previously only STFC staff could edit the Drupal sites but following requests from some projects a process is now in place to address this.

Following a recommendation from the Steering Committee to raise awareness of the Programme, work to relaunch it under a new name, logo, and website, is underway. A joint EPSRC-STFC press release is being developed to announce the relaunch of the Programme under the name "Computational Science Centre for Research Communities".

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

(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 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 Reseach 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.

Staffing	**Effort (FTE)**
Mark Forster	~~0.20~~ 0.05
Damian Jones	0.70
Viliam Kalavsky	0.50
Marion O'Sullivan	0.25
Barbara Montanari	~~0.20~~ 0.50
RIG Group	0.25
Total	**2.25**

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 450 UK members and over a 1000 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.

The 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 and over 500 google scholar citation in 2016. 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 chemoinformatics 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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Networking and Impact activities

The CoSeC work plan as described in the funded CCP5 proposal consists in a considerable amount of software development and maintenance as well as support for the rich programme of networking activities, public engagement, specialised workshops facilitation and training of the community via the DL_Software inititive. The tasks are progressed by all CCP5 funded members at Daresbury with John Purton leading the overall organisation as a CCP5 secretary. The following targets are planned with an indication of progress and persons involved:

- Organisation and support for the AGM conference in September 2016 at Harper Adams University (Loughborough could not manage it). John Purton organiser ongoing
- Organisation and support for training workshops for DL_Software. We expect to hold at least two major events lasting at least 2 days with one or two Hack Days at the back of these. This involves 3-5 Daresbury staff teaching and practical tutorials all of which require the continued development of training materials. In addition Daresbury staff handle the registrations and any associated fees, though additional help can be given to the local organisers as needed.
    - NSCCS, Imperial College, 18-20 April, 18 trainees over 2 days and 7 for the Hack Day (ITT, CY, MS, AE - HC, TY - ISIS)
- Organisation, lecturing and tutoring of the CCP5 summer school, which will take place at Lancaster during July (John Purton organiser and lecturer, Michael Seaton lecturer)
- Involvement in the organisation and delivery of CCP5 modelling outcomes and software for experimentalist and industrialist – November at Diamond (John Purton organiser, Ilian Todorov, Michael Seaton, Tom Keal, Chin Yong + CCP5 and BioSim heads)
- Involvement in the organisation of a joint conference with CCPBioSim "2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems", 13th-15th April 2016, Manchester.
- Plans for organising cross CCP workshop – CCP5/CCPi/CCPN(C)/SuperSTEPM on atom probed tomography, possibly summer 2017 (John Purton and others)
- Facilitate and organise the CCP5 visitor program
    1. Yethiraj – Wisconsin Q2 2016 (Paula Carbone, Manchester)
    2. Ignacio Pagonabarraga – Barcelona Q2 2016 (Michael Seaton, John Purton)
    3. Martin Schoen Q3/Q4 2016 (Henry Bock, HW)
    4. Mark Tuckerman – New York Q1 2017 (Ilian Todorov)
    5. Organized Prof. Ciccotti for autumn 2016, but he kindly agreed to speak at the AGM (John Purton)
- Development of outreach material and software workflow templates. (Chin Yong led, all Daresbury to contribute)
- Advertising of and administration of applications for student bursaries.
- Manage transfer of legacy to the new website server for http://www.ccp5.ac.uk (Chin Yong led, all CCP5 funded project leaders to contribute – Q2)
- Organise and publish outreach material on the new website (Chin Yong led, all CCG staff to contribute)
- Collection of impact data (John Purton responsible for delivery)
- Administration of membership list and email lists (John Purton, Chin Yong - ongoing)

DL_MONTE development and support

DL_MONTE is an atomistic Monte Carlo suite of techniques currently funded for fast track development by EPSRC as a CCP5 flagship code with developers at Daresbury (1) and Bath (2). On

CCP5 the project will provide continued support and collaboration with the community. Planned work under CCP5 includes:

- Improvement in the user manual, especially the introduction of more tutorial style material and discussion of test cases.
- A DL_MONTE workshop separate form DL_Software in early 2017.
- HPC work - there have been large structural changes to the code as part of the flagship grant. It is anticipated that only minor releases will be issued as bugs are fixed and ongoing internal modifications/improvements to the code are implemented.

The target for these plans is 0.29 FTE led by John Purton with extra 0.5 FTE for CCP5 administration.

ChemShell QM/MM development and support

Chemshell is a QM/MM project creating an stand alone environment to facilitate QM/MM practitioners with interfaces to many QM and MM programmes. The project will continue to maintain the Tcl-based version of ChemShell (v3.x) for the use of the CCP5 community while ChemShell undergoes redevelopment to a Python-based code. Support for the redevelopment is provided by external grants and the Materials Chemistry Consortium (see elsewhere in this plan), while CCP5 support is targeted at the Tcl-based release. Specific targets for CCP5 support include:

- Revision of the Tcl-ChemShell tutorial based on experience of previous ChemShell workshops, especially further QM/MM examples developed for the workshops.
- Release of ChemShell v3.7

The target for integration of DL_FIELD into Python-ChemShell referred to in the original draft plans has been deleted due to reduction in effort from the originally planned 0.15 FTE. The project is led by Thomas Keal (0.08 FTE)

DL_FIELD development and support

DL_FIELD (DL_ANALYZER) is a software project that aims to facilitate the rest of the CCP5 software projects and thus enhances their impact to the community and beyond. It provides access to system models used in the design and build up of bio-chemical, organic and generally soft-matter materials systems by producing the necessary input files needed for DL_POLY, DL_MONTE and DL_MESO. It also provides functionality aimed at solid state materials and can be used to design and build up organic-inorganic interfaces. The 2016-2017 planned work is summarised as follows:

- Extension and introduce DLF Standard Notation to other force field schemes such as CHARMM, CVFF, etc
- Restructuring program to reduce memory usage and improve efficiency in parameter data reading and storage.
- Introduce calling and mixing multiple potential schemes capability, including inorganic force field.
- Setup united atom model force field schemes.(for MMM activities)
- Multiscale work flow activities (multiscale materials modelling – MMM):
- Setup and running simulations – SDS as a case study – DL_FIELD-DL_POLY.

The project work together with website support and DL_Software workshops organisation is led by Chin Yong (0.81 FTE)

DL_MESO development and support

DL_MESO is a meso-scale software project that provides access to two methodologies for chemical applications on an engineering scale – DPD (bottom up) and LBE (top-down). Support for DL_MESO's LBE code is provided by UKCOMES, while CCP5 support is targeted at the DPD code. Planned developments for 2016-2017 on the CCP5 support include:

- Smoothed Particle Mesh Ewald (SPME) electrostatics model
- Tabulated potentials and thermostat screening functions (for MMM activities)
- Widom insertion for chemical potential calculations
- Code optimisations related to OpenMP multithreading, vectorisation and more efficient I/O

- Release of DL_MESO version 2.7

of which the inclusion of SPME and the release of DL_MESO version 2.7 are scheduled milestones. The project work is led by Michael Seaton (0.1 FTE)

DL_POLY development and support

DL_POLY_4 provides access to particle dynamics techniques; MS, MD, DPD with a range of user tools implemented as optional functionalities. DL_POLY is the largest software project at CCP5. Support and training to DL_POLY is currently funded by MCC by Ilian Todorov with the wide function of supervising new developments in DL_POLY and providing support as well as generating impact by publications and presentations at national and international conferences. At the present the DL_POLY project is recruiting.

CCP5	Milestone	Target Date
John Purton	Release of DL_MONTE2 *Task complete: the release of DLMONTE2 was delayed to Q2 2016. A second release was in Q3 2016*	Q1 2016
John Purton	Successful completion of summer school *Task complete*	Q3 2016
John Purton, all	Successful completion of AGM *Task complete: took place on schedule in September 2016 at Harper Adams University*	Q3/4 2016
Tom Keal	Update of ChemShell tutorial *Task complete: tutorial revisions are ongoing; revisions were completed following feedback from the DL_SOFTWARE ChemShell workshop in December 2016 and the tutorials were further revised for the workshop held in May 2017.*	Q1 2017
Tom Keal	Release of ChemShell 3.7 *Task complete: all technical developments are complete and the software is ready for release, which will be co-ordinated with the (LS) Dalton release in Q3 2017.*	Q1 2017
Chin Yong	Release of DL_FIELD 3.5 *Task complete: released on April 2016, together with manual updates*	Q2 2016
Chin Yong	Multiple potential capabilities in DL_FIELD including inorganic. *Task complete: only works for PDB structures*	Q4 2016
	Release of DL_FIELD 3.6 *Task complete: slightly ahead of schedule including manual updates in December 2016 to coincide with the DL_Software training*	Q1 2017
Michael Seaton	SPME in DL_MESO *Task complete: delayed slightly to Q3 2016*	Q2 2016
Michael Seaton	Release of DL_MESO 2.7 *Task in progress: completion will be Q3 2017.*	Q1 2017

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 2016 – 31 March 2017)

The effort provided in 2016-2017 was at a 1.93 FTE level, which was short of the planned level due to difficulties in recruiting. The shortfall of effort and recovery to plan was managed by a series of recruitments (July and November 2016) and resulted in two appointments – Vladimir Sokhan and Ivan Scivetti. This will result in an above average effort deployment from 2017/18, following a below average effort deployment during the first two years of this SLA cycle. Overall, during the course of the SLA cycle, we plan to deliver the full amount of support awarded to CCP5.

Due to the lower level of available support during 2016/17, priority was given to the preparation and delivery of two DL_SOFTWARE training workshops, CCP5 Summer School, CCP5 AGM and CCP5/CCPBioSim conference, as well as preparation of outreach material, a new website (launched) and over six invited presentations in the UK and overseas. Networking also proceeded as planned – events, opportunities, bursaries, inviting international visitors – without interruption.

Software plans and in particular project releases were rescheduled without interruption of business as usual service for all active software projects – funding, email, support and download. Support and development work on DL_FIELD, DL_MESO, DL_MONTE and ChemShell proceeded to plan and DL_POLY project plans will be fulfilled by the new starters.

The new "Simulations for the Experimentalist and the Industrialist" event (organised by John Purton, Ilian Todorov and Neil Allan, the CCP5 Chair) was held at the Diamond Light Source on 15-16 November 2016 and was a success. This event was fully subscribed (25 attendees) and well received by ISIS, Diamond, international institutions as well as commercial companies (Syngenta). Representatives from CCPBioSim, HEC-MCC, UCL, Diamond and ISIS, gave presentations at this event. The DL_Software Training and Hack Day at Daresbury Laboratory, 5-7 December 2016, attracted 25 participants from the UK and overseas. The CCP5 flagship program for atomistic Monte Carlo modelling, DL_MONTE, released version 2.03 in February. Prof Mark Tuckerman from NYU started his UK tour as an international CCP5 visitor in March 2017. The tour concludes in May 2017.

In March 2017 extra flagship development support was awarded by the EPSRC e-Infrastructure call in July 2016 and funds a PDRA at Daresbury and one at Bristol for 2 1/2 years.

A new opportunity has its origin in response to user requests from the University of Liverpool. A workflow combining DL_POLY, DL_FIELD & DL_ANALYSER has been used to demonstrate the integrated capability of molecular simulation software infrastructure to investigate quickly the detailed atomistic interaction behaviour of small gas molecules in organic binary solvents. A preliminary report led to a successful PhD studentship award at Liverpool. The future PhD candidate will be jointly supervised by John Satherley, David Cooper at the University of Liverpool, and Ilian Todorov and Chin Yong at STFC Daresbury Laboratory.

The successes and flexibilities of DL_Software have been demonstrated in the ADDoPT project (WP4 led by Kevin Roberts of University of Leeds) through a series of presentations and meetings. This led to an important decision to include DL_Software as the principal software infrastructure for molecular simulations.

We have had preliminary discussions with CCP_BioSim about running a further joint conference on Multiscale Modelling following our very successful joint meetings on this theme in 2014 and 2016.

A new CCP5 website came online after restructuring of the previous content within a new Drupal Content Management System hosted on virtual Apache server based at RAL. The content creation work was mainly carried out by Chin Yong.

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

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

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. JAP is responsible for organising the event alongside a local organiser and this year will take place at Lancaster University. JAP will lecture and coordinate the afternoon practical sessions and will MS 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.

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

FY 17/18 Staffing	Effort
John Purton	0.79 FTE
Chin Yong	~~0.59~~ 0.31 FTE
Michael Seaton	0.10 FTE

Thomas Keal	~~0.08~~ 0.20 FTE
Vlad Sokhan	1.00 FTE
Ivan Scivetti	1.00 FTE
Ilian Todorov	0.00 FTE
Total	**~~3.56~~ 3.4 FTE**

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

The main activities we plans to undertake during FY 2016/17 are:

Administrative and Scientific Support

- Leon Petit is CCP9 secretary and director of the Hartree CECAM node
- The group is responsible for the Psi-k and CCP9 web pages.

Web Material: Development and maintenance of the Psi-k web pages (psi-k.net) and CCP9 (http://www.ccp9.ac.uk),

Conferences/Workshops: Co-ordination of the programme of CCP9 Hands-on Courses. Organization of the biennial CCP9/Psi-k/CECAM Graduate School. Training courses will be delivered at a number of events including 'Physics by the Lake'.

Core Support Activities

A) Verification and Validation (V&V)

The aim is to compare systematically the accuracy of the full potential DFT part of Questaal (https://www.questaal.org), with that of other all-electron and pseudopotential DFT implementations. Implementation of a new fully relativistic core solver is planned as part of this effort. The goal is therefore to generate a module that is capable of switching between different modes, and to interface with electronic structure codes. This will result in much improved control over the output of different codes during verification, and increased confidence in the codes that use a well tested and verified module. This activity will include benchmark calculations with all-electron codes in the solid-state, to be used to verify pseudo-potential tables, and to benchmark different codes in a database. These activities will be carried in collaboration with CECAM's working group on 'Electronic structure verification and validation'. Subtasks are: (i) Perform calculations and filling the database; (ii) Discussions with CECAM V&V group; (iii) Implement flexible atomic solver in the FPLMTO code

B) Support of community codes

The planned subtasks are: (i) Support for the full potential linearized muffin-tin orbital (LMTO) code LMF, developed by Mark van Schilfgaarde**;** (ii) Support for the quasi-particle self-consistent GW code (QSGW) code, developed by Mark van Schilfgaarde**;** (iii) Support of the multiple-scattering code HUTSEPOT**;** (iv) Support of the CRYSTAL code; (v) Support of the KKR-DLM code developed by Julie Staunton

C) Novel materials

We will capitalize on our extensive modelling expertise for technologically relevant materials such as functional oxides, lanthanides, and actinides, to embed into community-codes the sophisticated correlated-electrons technologies that we have developed in the past two decades and that are required for quantitative predictions of the finite temperature magnetism or the electronic ground state of rare earth materials. In particular, this includes the self-interaction corrected (SIC) local spin density approximation, and the coherent potential approximation for disordered systems. This work will consist of the following subtasks: (i) CCP9 Flagship support: assist Mark van Schilfgaarde with making the QSGW method more efficient for large systems; (ii) Methodological developments; (iii) Code development; (iv) Demonstration and dissemination projects on specific compounds.

D) Workshops, Courses

Implementation of the programme of workshops, training courses and conferences, i.e. the activities funded under the existing CCP9 networking grant and the additional networking activities described above. Ongoing activities include the coordination of interactions with academic and industrial partners, and the coordination of CCP9 (hands-on) training courses

E) Support of the Psi-k network

The ongoing tasks carried out for the Psi-k network include: (i) Arranging and publishing Psi-k scientific highlights; (ii) Providing administration and content support for the new Psi-k web portal psi-k.net; (iii) Running the Day to day management of the Psi-k charity, report to Charity Commission.

CCP9	Milestone	Target Date
	SIC-LSD rare earth pnictide/chalcogenide review article *Task complete: article published.*	Q2 2016
	Rare earth doped ceria article *Task ongoing: calculations are done but LP is focussing on other papers with Julie Staunton that will be added as new tasks in the 2017-18 plans.*	Q2 2017
	Workshops: a) State of art electronic structure b) CCP9/CECAM/Psi-k school *Task complete: both workshops were successful.*	Q3 2016
	Flexible atomic solver module implemented in FPLMTO *Task complete: Jerome Jackson has completed this work with van Schilfgaarde. The atomic solver module has been updated and the work is now complete. Jerome will write a report on the work.*	Q1 2017
	Collaboration with Julie Staunton on permanent magnet materials first results *Task complete: LP has produced some results with Julie Staunton's PostDoc and has also visited AMES. A paper has been submitted to the Journal of Magnetic Materials and is currently being refereed. Leon is also working on a more extended article for PhysRevB and has started some collaborations with India following a visit to a conference earlier this year. A couple of projects have been started and may result in new tasks for next year.*	Ongoing
	V&V for the elements *Task complete: Jerome discovered a number of bugs which have now been fixed. Jerome will now move on to the rare elements as a new task.*	Q1 2017
	KKR hands-on course *Task complete: Took place in November 2016 with 24 attendees.*	Q2 2016

	Article on actinide-oxides *Task in progress : the article will be on transition metal oxides and will be delayed until later in the year as other tasks have taken preference.*	Q1 2017
	New CCP9 Webpage *Task complete: new website went live in January 2017.*	Q1 2017
	Implementation of SIC in LMF; initial phase *Task complete: the initial phase work is now complete Jerome has presented the work in Lund, Sweden.*	Q1 2017
	Crystal code *Task complete: the latest version of the code has been uploaded. A more descriptive task has been included in next year's plans for this action.*	Q1 2017

Staffing	**Effort Funded**
Leon Petit	1.00 FTE
Martin Lueders	0.20 FTE
Barry Searle	0.38 FTE
Jerome Jackson	1.00 FTE
Total	**2.58 FTE**

CCP9 – Summary Report (1 April 2016 – 31 March 2017)

Research on correlated electron systems: The theory-experiment collaboration with Julie Staunton (Warwick University) and Ames Laboratory (US) is on-going. The goal of this collaboration is the development of novel magnetic materials. Our initial findings on Gd-intermetallics have recently been published in Physical Review Letters, a follow-up article has been submitted to Journal of Magnetism and Magnetic Materials, and an extensive article which includes our latest work on the magnetism of alloys, is in preparation. Furthermore, in the framework of our collaboration with Warwick University, we have started investigating Fe3O4 and GdCo5 for their potential use as spintronics materials and permanent magnets respectively.

A topical review on selected rare-earth compounds, was written following an invitation by Institute of Physics, and has now been published in J. Phys.: Condens. Matter

Support on the Flagship Project: the current CCP9 flagship grant is focussed on the suite of codes Questaal (https://www.questaal.org), and seeks to overcome the limitations of the widely used Density Functional Theory (DFT) when it comes to describing many body effects. Observables that are particularly sensitive to the accuracy of this description are the electronic properties of semiconductors and excitation spectra. This work is therefore expected to improve significantly the predictive power of modelling and simulation of properties relevant for electronics applications. The code implements a Green's function based approach, known as GW, in both its one-shot and self-consistent forms. Recently, the GW has been redesigned for greater efficiency; a large part of this development was done by Martin Lueders, partially funded by an embedded CSE award from the Edinburgh Parallel Computing Centre. Further improvements have been implemented as part of the flagship support. Quasi-particle self-consistent GW calculations can now easily be done for systems with 30 to 40 atoms.

The validation and verification work: One of the most important developments of the electronic structure field in the last few years has been the emergence of careful verification of solid state codes within the Delta-Codes project [Science 351, 2016]. Joining this effort, a detailed verification process is underway (by Jerome Jackson), where the accuracy of the full potential DFT code (part of Questaal) has been systematically compared with that of other all-electron and pseudopotential DFT

implementations. The work has led to the identification of a number of issues limiting the accuracy of the code compared to other high-accuracy codes. It has motivated the development of a new fully relativistic core solver, together with identifying and fixing a number of implementation problems. The final results will shortly be uploaded to the Delta-Codes website.

Calculations extending the Delta-Codes test cases to include the lanthanide elements have been completed, and it is envisioned that these will be compared with CASTEP calculations, once a specification for reaching highest accuracy has been proven.

CRYSTAL electronic structure code: A small amount of effort in support of CCP9 is devoted to the CRYSTAL code and contributes to the bulk of the work, which is performed in support of the Materials Chemistry Consortium (see the related section for details on the CRYSTAL code). Specifically for the CCP9 community, a number of bugs were fixed, and the current developer version of code has been merged with the master code from Italy. CCP9 is responsible for maintaining the UK CRYSTAL repository on CCPForge. Initial results for the Validation & verification of the CRYSTAL code have also been obtained.

The new CCP9 webpage has been built using the Drupal content management system, and is now live. Among others, the next steps will include reorganizing the working groups.

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. Three highlights were refereed (including one with Martin Lueders as co-author) and edited during the reporting period, and submitted to the mailing-list which now reaches more than 3000 people.

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

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

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.

Staffing	**Effort Funded**
Leon Petit	1.00 FTE
Martin Lueders	~~0.7~~ 0.20 FTE
Jerome Jackson	1.00 FTE
Total	**~~2.7~~ 2.20 FTE**

The funding reprofiling is likely to result in a new recruitment during this year or the next.

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.

Our support is focussing on bridging the codes for different length scales and to provide computational support for users of the ISIS neutron scattering facility.

CCP-mag – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Administrative and Scientific Support

- Serve as CCP-mag secretary
- Development and maintenance of the CCP-mag web pages (http://www.CCP-mag.ac.uk)

Core Support Activities

A) Implementation of common I/O routines and Support of community codes

In collaboration with the main developers of the codes, implement I/O routines for the data sets in the decided data format.

B) Support of ISIS community codes

The core support team will assist ISIS to integrate their codes more closely into the ISIS workflow environment, and also interface the codes with codes used for the interpretation of magnetism-related experiments.

C) Workshops, Courses

Implementation of the programme of workshops, training courses and conferences. Ongoing activities include: (i) Coordination of interactions with academic and industrial partners; (ii) Coordination of CCP-mag (hands-on) training courses.

CCP-mag	NMAG installation procedure *Task complete: Discussions are in progress about providing CI tools to Hand Fangohr (Southampton).*	Q2 2016
	Co-ordinate session at IOP Magnetism 2016 *Task complete: Leon Petit and Julie Staunton attended. Not an explicit session for the CCP because people were distributed in other sessions.*	Q2 2016
	Organise Computational Magnetism Session at Temm 2016 *Task complete: a session was organised with four speakers.*	Q2 2016
	Discuss the possibility of a flagship proposal	Q2 2016

	Task complete: a proposal was submitted with Richard Evans and Julie Staunton which was unfortunately rejected.	
	Organise SpinW course *Task complete: took place at RAL in February 2017 with 20 attendees.*	Q1 2017
	Run KKR course (joint with CCP9) *Task complete: course took place at Daresbury, November 2016.*	Q4 2016
	Discuss integration of KKR with ISIS codes *Task complete: Martin visited Budapest where discussions took place.*	Q4 2016
	Implementation of I/O routines for common data *Task ongoing: in agreement with the CCPmag Chair, effort will be concentrated on this task from FY 2018/19*	Q1 2017
	Plan computational magnetism session for TEMM 2017 *Task complete: 2 speakers slots available for CCPmag community on the agenda. Funding from CCP-mag was not used for this workshop and will now be diverted to the IOP Magnetism meeting instead where there will be 2 sessions specifically for Computational Magnetism. Martin has emailed the community asking who would be at the IOP Meeting. There will be a CCP-mag meeting during the event to discuss future involvement.*	Q1 2017

Staffing	**Effort**
Martin Lueders	0.25 FTE
Barry Searle	0.3 FTE
Total	**0.55 FTE**

CCP-mag – Summary Report (1 April 2016 – 31 March 2017)

The Theoretical and Experimental Magnetism Meeting (TEMM) is one of the main meetings of users of the ISIS neutron scattering facility with an interest in magnetism of correlated materials. In accordance with the work plans, a Computational Magnetism Session was organized at TEMM 2016 in order to bring the ISIS community together with the computational magnetism community. The speakers were selected from the CCP-mag community (Bob Stamps, Gino Hrkac, Leon Petit) and from abroad (Tom Ostler, Liege, Belgium). During the TEMM and also other follow-up meetings, the possibility of a new CCP software development flagship proposal was discussed. Richard Evans (PI) and co-workers submitted a proposal to further develop the VAMPIRE (atomistic spin modelling) code. The proposal was not funded.

Discussions have been held with Toby Perring (ISIS neutron facility, RAL) about integrating the first principles electronic structure codes for calculating spin excitations into the ISIS software platform MANTID, a framework that supports high-performance computing and visualisation of materials science data (https://www.mantidproject.org). A pilot project funded by STFC is underway to compute magnetic excitations of simple metals. The main outcome of this project so far is that further development of the functionality to compute magnetic excitations is needed before fully automated calculations are possible. A grant proposal is being discussed involving Toby Perring, Keith Refson, Martin Lueders and Dominik Jochym (CoSeC support for UKCP).

In order to facilitate true multi-scale calculations of magnetism, results from the quantum scale need to be fed to the next level, for instance as input parameters in atomistic spin model calculations. Ad hoc calculations, where the data is transferred by hand, have already been performed by a collaboration of the York group and Laszlo Szunyogh's group in Budapest. Discussions with the

working group on how to automate the process resulted in the decision to join forces with a CECAM activity on a electronic structure common data format (ESCDF). This format, which is being drafted by the CECAM Electronic Structure Library (ESL) activity in conjunction with a European COST network on spectroscopy (EUSpec), will provide a common format for geometry information, as well as further quantities related to ab initio calculations. The underlying framework can easily be extended to include magnetic properties such as exchange interactions. As this ESCDF library will be of significant value for the CCP-mag community, the working group agreed to invest some of the core support for the development of this library. To further this project, Martin Lueders co-ordinated a meeting with Laszlo Szunyogh in Budapest, which was also joined by members of the CECAM ESL activity.

Further discussions with members of the working group showed a need for a systematic study of the reliability of ab initio calculations of magnetic exchange interactions. This activity is currently being discussed as a likely candidate for the 2018/19 CCP-mag CoSeC work plan.

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

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

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.

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

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. The aim is to cement the strong interaction between experiment and computation of solid state NMR. The project will greatly improve the visibility and efficiency of research activity in this area. It will provide the foundations to provide major impact across materials science and solid state, pharmaceuticals, supramolecular and geochemistry.

CCPNC – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Specifically the CCP exists to:

- Facilitate the interoperability of the range of simulation software used by the solid state NMR and crystallography communities providing overarching tools
- Provide support and enhanced functionality for solid state NMR users of first principles codes specifically a library of tested pseudopotentials with validation data; the ability to compute NMR spin-spin couplings and inclusion of relativistic effects for accurate calculation on heavier elements
- Develop a world-wide visible database of computed NMR parameters suitable for data mining

- Provide a central source of information on NMR crystallography software, providing links into existing resources where these exist
- Provide training at the PhD and PDRA level to a broad audience including those in the fields of Materials Science, NMR and Materials Modelling
- Develop the theory and computational tools to address the outstanding challenges of predicting NMR parameters for paramagnetic systems with exemplar calculations on materials for Catalysis and Li-ion batteries
- Provide a focus for the UK community involved in NMR Crystallography to engage in European Projects for example through partnerships with CCPN, CECAM, SMARTER conference series
- Develop protocols and tools for the interoperability of the different software elements as well as expanding their functionality where appropriate. For each class of software there are often several codes available. For spin-simulation software a number of well-developed programs exist. At the ab initio level CASTEP is widely used in the UK. However, the full potential Wien2K code is currently developing NMR functionality (in close collaboration with members of this CCP). It is not the intention of CCP-NC to impose a unique software choice: rather CCP-NC will promote workflows and tool chains.
- By establishing standardised file formats and benchmark datasets it will be possible to interchange individual components with a workflow for example performing spin simulations with either SIMPSON or pNMRsim.

This will include work on:

- First principles simulation
- An archive format for calculations of magnetic resonance parameters
- Database of NMR parameters
- Interface from first principles to spin simulation programs
- Interface to crystallographic software

CCPNC	Milestone	Target Date
	Joint organisation of CASTEP training workshop *Task complete: workshop took place in August 2016 with seventy attendees for five days.*	Q3 2016
	Development of new tools for integration of XRD spectroscopy results with NMR crystallography *Task ongoing: current work is moving in a different direction. This task may no longer be relevant – to be confirmed.*	Q4 2016
	Development of Python library for complementing Random Structure Searching with NMR crystallography *Task complete: NMR functionality has been added to the library, as well as new functionality for remote submission of jobs to HPC machines, and version 0.6 has been publicly released on CCPForge.*	Q1 2017
	Preparation for release of Nuclear Independent Chemical Shifts (NICS) tool “current2nics” for CASTEP *Task complete: the preparation work has been done.*	Q3 2016
	Joint organisation of advanced NMR-CASTEP workshop *Task complete: this workshop was cancelled by the co-organisers at Oxford and will not take place.*	Q1 2017

	Setting up database for NMR parameters *Task complete: Albert has set up a prototype for the back-end of the database, and Simone has worked on options for the front end. This has been presented to the CCP-NC committee and work to draft the requirements of the interface that will be implemented in the final version is ongoing through discussion with the rest of the supported community*	Q1 2017
	Submitting a paper on using Machine Learning to compute NMR parameters in amorphous silica and glycine *Task ongoing: this paper will be submitted by Albert Bartock-Partay.*	Q1 2017

Staffing	**Effort**
Simone Sturniolo	1.00 FTE
Albert Bartok-Partay	0.50 FTE
Total	**1.50 FTE**

CCPNC – Summary Report (1 April 2016 – 31 March 2017)

Effort has been provided by Simone Sturniolo and Albert Bartok-Partay, who joined the project in October.

One of CCP-NC's first projects has been the development of MagresView, a visualisation software enabling experimental scientists to plot and manipulate the raw data produced by simulations in a very intuitive and accessible way. It helps them to visualise NMR data computed ab initio, by representing them as 3D graphic elements directly on the chemical structure of the compound of interest. The software works on all major browsers for Windows, Mac OS and Linux and has minimal requirements to make it quick and easy to use.

Following on from the release of the software a few years ago, a paper has now been published introducing it officially to the worldwide community and providing a reference point for those wishing to use and cite it. The software is now at a mature stage and during the reporting period only routine maintenance was needed, leading to the release of version 1.6.2.

A companion tool, the Soprano Python library, has been released in alpha status on CCPForge for public use. One of the most common techniques for the automated search of new crystal structures is Ab-Initio Random Structure Search (AIRSS), consisting of creating a number of potential candidate structures at random to then optimise them with ab-initio quantum chemistry simulation software and classify them based on their final energy. Soprano was born as a tool to enhance the classification process, by allowing us to manipulate thousands of structures in complex ways, assessing a number of geometric or chemical parameters and grouping them by similarity. It has now moved beyond just that and provides all-around functionality for work with small databases of chemical structures. During the reporting period, work was focused mostly on inclusion of the new NMR specific functionality, which allows manipulation of Magres data similar to the one provided by MagresView as well as more advanced spectral simulations that include powder averaging effects.

There is a growing demand for a database of computed NMR parameters, partially as a repository of original research data, but also serving as a resource for reference data, which enables data mining as well as minimising the need for repeating calculations. A prototype of a database of NMR parameters of inorganic materials based on the Inorganic Crystal Structure Database has been set up. This will be used to gather feedback on its usage from a set of test users, and this knowledge will in turn be used to develop a public repository.

A different strand of work relates to the computation of NMR parameters using first principle quantum mechanical calculations. In general, this is well established and has excellent experimental validation. However, there are a few classes of compounds, such as fluorine-containing materials, where such predictions are systematically less accurate. The relatively new modified Becke-Johnson exchange potential, which should provide a better approximation in these cases, has been implemented in a development version of CASTEP and is now in the alpha testing stage. It should be noted that this new development will be useful to CASTEP users generally, beyond the communities we directly support. This includes other EPSRC SLA supported communities such as CCP9 and UKCP.

Even though NMR parameters can be routinely computed, calculations are still relatively expensive and limited to a few hundred atoms at most. A possible way to accelerate these calculations is to utilise Machine Learning techniques, which would fit computed NMR parameters of crystalline structures. Work in this area is being started which, if successful, could bring a brute force approach to experimental NMR crystallography searches, which identify the structure corresponding to a certain set of measured parameters, into the realm of practical possibility for at least some families of compounds.

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

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

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.

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

CCPQ – Quantum Dynamics in Atomic Molecular and Optical Physics

The overarching aim of 'Collaborative Computational Project in Quantum dynamics' (CCPQ) is to facilitate theoretical atomic, molecular and optical (AMO) physics in the UK by developing, curating and disseminating software for describing coherent quantum dynamics and interactions of particles. Its work is aligned to EPSRC physical sciences and Quantum Technologies themes in the areas of "chemical reaction dynamics and mechanism", "antihydrogen", "light-matter interaction and optical phenomena", "cold atoms and molecules" and "photonic materials". All are areas of fundamental

science that underpin emerging technologies which use light. New experiments and facilities such as free electron lasers, ultrafast dynamics experiments, ultracold atoms in optical lattices, ion trapping and the anti-hydrogen experiments at CERN, mean that AMO physics is a rapidly expanding field. There is also a continual need for more sophisticated atomic and molecular collision and resonance data for studies of industrial plasmas, astrophysical plasmas, nuclear fusion reactors, atmospheric physics and investigations of the effects of electron (and positron) collisions with molecules in cells. CCPQ supports the development of community codes in a number of related areas: electron collisions, anti-matter, quantum information, attosecond physics, molecular wavepackets and ultra-cold molecules. New and upgraded maintained software is required so that the UK can retain its leadership in this area. CCPQ and its parent networks CCP2 and CCP6 have been in existence since ~1978. The current CCPQ network is directed by a Steering Panel chaired by Professor G Worth (UCL) with deputy chairs Professor H van der Hart (QUB) and Dr Stephen Clark (Bath): the full range of the panel and wider working group may be found at https://www.ccpq.ac.uk/AboutUs. Core support allocated to CCPQ is 2FTE, effectively 1.86 FTE with 7% taken for central CCP SLA support. The project is supported by the members of STFC SCD's Theoretical and Computational Physics Group (Martin Plummer), the Applications Performance Engineering Group [now the Hartree Centre HPC-Software Engineering Group] (Andrew Sunderland) and the SCD Software Engineering Group (SEG, S Lamerton and C Jones). SEG has been providing sustainability, testing and best practice support across CCPQ's project groups.

CCPQ – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Martin Plummer provides scientific and optimization/parallelization support to the R-Matrix electron-atom collisions codes PRMAT/PFARM, which also act as starter codes for CCPQ's (ultrafast pulse) laser-atom code RMT, and as a long-term core support project is developing double-electronic-continuum theory and coding (to eventually be applied to RMT and the intermediate energy collision code 2DRMP) as modifications of PRMAT. Andy Sunderland (with MP) provides coding, parallelization/optimization support for PFARM and the electron-molecule codes UKRMol/UKRmol+. AGS (and MP) will continue to provide expertise in novel technology code developments following the successful collaboration will ICHEC Dublin on Xeon-Phi optimization of PFARM. MP provides support for MM Law (Aberdeen) and EAG Armour (Nottingham) on low-energy antimatter collisions relevant to, for example, the CERN ALPHA project. Currently the Oxford/Bath TNT (tensor network analysis for strongly correlated systems) group prefers more general software engineering and 'outreach through software' support that SEG provides, and the possibilities that STFC's planned upgraded website software and management can provide. SEG/SESC will continue to expand its continuous integration environment with specific CCPQ assistance for the network's codes.

CCPQ	Milestone	Target Date
Atomic R-matrix:	Review/testing of new general double-continuum inner region static codes with respect to community codes RMT (time dependent laser atom) and 2DRMP (time independent collisions). *Review/testing of the static inner region R-matrix codes DONE. Extra coding for specific double-continuum applications is underway (this is the most complex coding project for MP's core support and is being approached as rigorously as possible).* Revise theory paper as required, begin preparation of follow up code description paper/manual *Paper revised and rewritten/expanded to incorporate additional features relevant to the multi-domain 2DRMP code in particular, and to improve the rigour and clarity of the mathematics. Code description is being generated as the code is developed.* Support for eCSE proposals and for EPSRC Flagship proposal. *Complete: QUB/OU Flagship for RMT/UKRmol+ was funded.*	Staggered milestones throughout year. eCSE: Q2-Q4, Flagship: Q3-Q1

	Complete comparisons of PFARM with QUB (C Ballance) code PSTGF. Consider further comparisons on new targets, to check accuracy against reliable PFARM results. *Initial set completed, new set postponed as QUB concentrated on a (successful) grant application (in addition to the Flagship).* AGS/MP: Continue novel technology collaboration with ICHEC and practical extension to other codes. *Task in progress with additional DL collaboration through PRACE. AGS also assisted with novel technology details for the Flagship.* SEG: Agree future strategy for cross-platform management of atomic R-matrix codes: support RMT port to CCPForge. Translate CB's PERL R-matrix interface to Python. Discuss new work. *Tasks complete*	Q2 2016 Continuous, as per ICHEC availability Q2-Q4 2016
Molecular R-matrix	AGS to work on memory optimization of molecular collision code UKRMol+. Staggered objectives with in-year review *Initial tasks complete, new tasks agreed (complementary to a new UCL eCSE) and completed/on track. Plans for 2017-18 agreed MP and AGS also met UCL eCSE RSE Ahmed Al Rafaie and advised on shared-memory parallel optimization.* MP to work with OU PhD student on application of the TIMEDEL resonance code. MP, AGS (+ UCL) to revise TIMEDEL paper according to referee reports *Task complete: paper accepted by CPC.*	Q2, Q3, Q4-Q1 Q3 2016 (Q1 2017)
Antimatter	Advise MM Law, B Mant (Aberdeen) on their antihydrogen paper preprints, discuss next stage of support following B Mant's departure, possible joint discussions with Birmingham (Quantics). *Task complete.* MP to revise submitted annihilation paper as required by referees, background work (secondary to direct CCPQ requirements) on follow up positron work to be considered. *Task complete: paper published (background work ongoing)*	Q2-Q3 2016, Q1 2017 Q2 2016
Further SEG support for TNT, Quantics and UKRMol	SEG to agree with TNT the next level of support following completion (in Q1 2016) of the Python interface proof of concept. *Task in progress as agreed with collaborators: Steven Lamerton has met with the TNT computational scientist. Main plan is to upgrade the Python AP.I Owing to SL's sick leave and the new TNT RSE (Michael Lubasch) taking time to become familiar with TNT, this will resume in 2017-18.* Review of use/progess by all packages of the 'continuous integration environment' (CIT a.k.a. SESC Build Service) *Task complete: the initial review is now done.* Resolve in-year licence issues for UKRMol codes and continue CIT build of UKRmol. *INTEL licence issue has now been resolved by CJ. UKRmol CIT support was agreed as part of the Flagship proposal and will commence (separately/alongside SLA core support) in 2017-18.* Additional Build Service changes for Quantics and new tasks. *Task postponed: delay caused by Graham Worth's move to UCL. Tasks agreed for 2017-2018 (Q2-Q3) following SL's Q1 illness.*	Q3 2016 Q2 2016 Q3-Q4 2016 Q1 2017
Web Page and General	Following initial testing of the new STFC website technology, have a practical strategy and produce a modern vibrant CCPQ website. *Task complete (after some effort): website is now live and working*	Q2 –Q3 2016

	well. The TNT group were given web-admin support for the upcoming 'Windsor 2017' workshop. Allow steering panel members to upload content to website. Monitor use of 'live' website and any teething troubles *Done: approved external people may now edit the Drupal sites.*	Q3 2016

Staffing	**Effort**
Martin Plummer	1.00 FTE
SEG (mainly Steven Lamerton)	0.36 FTE
Andrew Sunderland	0.50 FTE
Total	**1.86 FTE**

CCPQ – Summary Report (1 April 2016 – 31 March 2017)

Work during the reporting period progressed smoothly, with milestones achieved or, if priorities changed, revised in agreement with CCPQ members. In addition to originally planned objectives, core support assisted with CCPQ's response to the EPSRC Flagship Call. Following an internal CCPQ proposal selection, the 'R-matrix' Flagship Proposal was submitted by H van der Hart (HvdH), Queen's University Belfast (QUB), with J D Gorfinkiel (JDG), Open University (OU), on ab initio laser-atom/molecule work 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. Code curation, rigorous testing and sustainability are highlighted as part of the Flagship development. Martin Plummer advised on future porting to novel technology, using ports of the 'PFARM' outer region code as examples, and will dedicate core support effort to the project. HvdH and JDG were successful, with the proposal ranked overall 2nd by the project panel.

The CCPQ website was relaunched by Martin Plummer. This required effort to make use of detailed Drupal (content tool) features, modernising various links and encouraging members to contribute summary introductions and visual content. Thanks are due to those who contributed and the site is in use and up to date with new resource pages planned for 2017-2108.

Scientific work on atomic R-matrix double-continuum theory and code continued, with a 'definitive' theory paper (mainly written by Martin Plummer) to be submitted in 2017 (the final draft is with co-authors at the time of writing). Work on UKRmol+ has continued, with A G Sunderland achieving and then extending strategies for significant memory optimization. The new stage of this work, with JDG and Z Masin (MBI-Berlin), is now being implemented. A code TIMEDELN for resonance detection (J Tennyson and D Little, UCL with AGS, MP) was published in Computer Physics Communications. Martin Plummer helped OU student A Loupas with TIMEDELN use and interpretation, and UCL eCSE PDRA Ahmed Al-Rafaie with UKRMol+ parallelism. A paper on resonance-enhanced annihilation of positrons by molecules was published (EAG Armour, Nottingham and MP); Martin Plummer also discussed drafts of antihydrogen collision papers (relevant to CERN experiments) by MM Law and B Mant (Aberdeen, UCL) with the authors and had initial discussions with MML for new work in 2017-18.

Steve Lamerton and Catherine Jones supported QUB, OU-UCL and the Tensor Network Theory (TNT, modelling strongly correlated systems as coupled networks of tensors) group at Oxford. The 'TNT Virtual Machine', allowing direct use of a training version of TNT without complicated installation issues, has been added to CCPForge. Steve Lamerton has met the new TNT PDRA Michael Lubasch (replacing S Al-Assam).

RMT was ported to CCPForge following restructuring (by QUB/MBI with advice from Steve Lamerton) and is updated daily from the RMT group's Gitlab base server. A Python script has been written for Dr

C Ballance (QUB) enabling users to download, set up data and tests/runs of his parallel electron-ion collision R-matrix codes.

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

(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 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.

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

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 28/5/2018.

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

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 maximising 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 maximise 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
	Benchmark and optimize new field calculation in GS2 *Task complete: this task has support from NAG and is looking at optimizing more widely. The original scope for this task has been met and a new milestone will be added to next year's plans for the new scope.*	Q2 2016
	Implement implicit timestepping in CCFE's BOUT++ physics module to allow timesteps comparable with ion timescales. *Task complete*	Q3 2016
	In GS2, implement collisions module using field solve memory layout to reduce memory redistributions. *Task complete*	Q4 2016
	In BOUT++, rewrite solver monitors to allow multiple monitors and extend their scope. *Task complete*	Q1 2017

Staffing	Effort
Joseph Parker	1.00 FTE
Short-term new recruit	0.48 FTE
Total	**1.48 FTE**

CCP Plasma/HEC Plasma – Summary Report (1 April 2016 – 31 March 2017)

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 the simulations of fusion plasma are computationally very expensive. GS2 is a plasma turbulence code which has been developed since the 1990's and is already highly optimized; however simulations still cannot resolve necessary space or time scales. In this reporting period, an in-depth performance profiling of the code was undertaken. This highlighted that the redistribution of data in memory was preventing the code from scaling to high core counts. Parts of the code were rewritten in a new memory layout to reduce data redistribution. This yielded a 30% speed-up at high core counts. Such performance improvements are valuable, as GS2 is regularly used for "heroic" simulations which use as high resolution as possible. Work on further reducing the redistribution of data is now ongoing.

The profiling was performed in collaboration with the Culham Centre for Fusion Energy (CCFE), the Numerical Algorithms Group (NAG) and the Oxford e-Research Centre (OeRC), through a Performance, Optimization and Productivity (POP) project.

Achieving fusion also requires an understanding of plasma behaviour at the tokomak edge. For such simulations to be accurate, they must incorporate the behaviour of both the electrons and the ions in the plasma. This requires the resolution of widely-separated scales in space and time. This reporting period, an implicit-explicit time-advance routine was implemented in STORM, CCFE's physics module for BOUT++, allowing small electron scales to be resolved while retaining the large time-step associated with ion scales. This yields a speed-up of a factor of 3 compared to STORM's current time-advance method.

The Odin project is aimed at developing a UK academic radiation hydrodynamics code for laser-fusion research. This will allow UK involvement in multi-billion dollar facilities in the US and France. This is a major project with 10 developers contributing from 5 institutes. Management of such a complex development project requires rigorous structures for code sharing. In this period Odin became sufficiently well development to have a major join release combining all Lagnrangian physics packages. To ensure the development runs smoothly much of the Plasma HEC supported PDRAs time over the last 6 months has been on building regression testing suites and documentation through Doxygen and MediaWiki.

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

(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.

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

CCPi – Tomographic Imaging

Non-destructive 3D X-ray, Neutron, PET and MR imaging are becoming increasingly important in many areas of science with application to Energy, Healthcare and Security. For example X-rays are having a dramatic impact on fields as diverse as security (e.g. baggage and body scanning at airports and screening of vehicles at ports), engineering (e.g. visualising stress corrosion cracking in nuclear plant and the degradation of fuel cells) and medicine (e.g. cancer treatment and artificial tissue engineering). The spatial and temporal resolutions are increasing dramatically. RC funded synchrotron sources are rapidly increasing the numbers of x-ray imaging instruments available (the European Synchrotron Radiation Facility (ESRF) now has 10 beamlines, and Diamond Light Source (DLS) is currently building 4 new imaging beamlines). Also laboratory x-ray imaging facilities are becoming increasingly widespread. This expansion is mirrored elsewhere with the global CT market now worth $150M (+ $5B in medical CT) both expanding at 10% per annum, while 30% of the data stored on the world's computers are now medical images. Unsurprisingly, papers on these tomography have also increased sharply this decade.

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. There are four major parts: pre-processing techniques for image calibration and noise reduction, reconstruction techniques to create a 3D volume data set from projections and segmentation, quantification techniques that can extract relevant objective values from these 3D volumes, and software framework development to enable the exploitation of CCPi codes in a wide range of existing commercial and open source software.

The size of this community has grown over the last five years with many academic groups around the UK taking up tomographic imaging and purchasing new lab based x-ray CT scanners. The size of our community has arisen from ~250 in 2013 to over 330 in 2017, over 30% growth in the last five years. In 2012 there was an estimated 50,000 CT imaging sources around the world.

Our focus is aiming at bringing together the UK imaging community, specifically to maximising the return on investment in imaging software development through developing, maintaining, and prompting the CCPi core imaging toolbox. 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.

CCPi – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Outline of Proposed Core Support Activities:

Most people who acquire and analyse images have little or no knowledge of the type of tomography reconstruction or analysis available; consequently the involvement of the STFC support is critical to achieve a significant step jump in the level of information obtained by UK science from X-ray and PET/MR imaging. As well as administrative support for all of the CCPs (organization of working group meetings, maintenance of web sites), the core support team will:

- Standardise input and output data formats;
- Standardise software coding rules and testing;
- Assist with porting, parallelisation and optimisation on different hardware platforms including novel architecture systems.
- Provide centralised distribution and controlled releases for software;
- Provide installation user support for software, and run workshops/training events;
- Collate and distribute existing algorithms and code, including licensing requests;
- Encourage CCPs participants to make their algorithms and code available;
- Create a gallery of test real image and volume datasets for mathematicians to test and benchmark new algorithms; and
- Maintain documentation.

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives *Task ongoing: website updated, tested and working.*	Ongoing
	Organise working group meeting and monthly joint show-and-tell sessions *Task ongoing: 37 show and tell events have taken place in the last three years. The last show and tell meeting took place in December 2016 and there was a group meeting in March 2017.*	Ongoing
	Support current training courses and organise developer workshop to teach *Task ongoing: Martin was the co-organiser for four training courses.*	Ongoing
	Embed framework: ISIS/IMAT *Task complete: phase one has been done and the project is now moving into phase two which will be a new task in the 2017-18 plans.*	Q2/3 2016
	Embed framework: DLS/savu *Task complete: phase one has been done. The CCPi code is in the framework and on SCARF. Phase two will be a new task in the 2017-18 plans.*	Q4 2016
	Embed lab based framework: UoM/ UoS/ UoW *Task complete: the framework is embedded. A new milestone for linking the SAVU framework will be included in the 2017-18 plans.*	Q3 2016
	Add quantitative code examples from the community *Task complete: a new release has happened. CCPi is targeting two or three code updates each year.*	Q4 2016
	Add pre-processing stages inc. beamhardening correction experiments at DLS. *Task complete: the work is complete and should be published in May 2017.*	Q2 2016
	Organise the main ToScA conference; September 2016 *Task complete: One hundred and forty people attended over three days.*	Q3 2016
	Optional: Iterative code for the Nikon XTek X-Ray CT accelerated versions (OpenCL, Xeon Phi) *Task ongoing: planning a workshop with co-investigators to work out how to link everything together that will take place in the next reporting period.*	Q1 2017
	Optional: Optimise OpenCL projection algorithms.	Q1 2017

	Task ongoing: the new recruit will be looking at this in the next reporting period.	

Staffing	**Effort**
Martin Turner	0.10 FTE
Ron Fowler	0.20 FTE
Sri Nagella	0.50 FTE
New Hire	0.45 FTE
Erica Yang	0.05 FTE
Total	**1.30 FTE**

CCPi – Summary Report (1 April 2016 – 31 March 2017)

In the reporting period, the core support effort (1.0 FTE) was provided by Sri Nagella, Ron Fowler, Martin Turner, and Erica Yang. We have re-profiled the work (~0.5FTE) from the reporting period to 17/18 FY. A new starter, Dr Edoardo Pasca, for CCPi has been successfully recruited to join the core support team in Feb. 2017.

Code inventory: The CCPi codebase has gone through a phase of rapid growth. As of January 2017, we have received codes and contributions from 12 code owners and 5 universities/organisations (DLS-1, Manchester – 9, Leeds – 1, Bath - 1) from the community with an estimated 50 algorithms. An additional three more codes from the community are pending for review. They not only demonstrate that CCPi has a strong community but also provide a testament of complex algorithmic and software development challenges faced by the community. The codes cover the entire experiment CT image analysis pipeline from pre- and post- processing, reconstruction, segmentation, through to quantification. The diversity and sheer number of the codes have triggered a code inventory review to enable the working group to prioritise the development needs and to review the CCPi toolbox framework design. In March 2017, a new brand for CCPi toolbox, namely CCPi Core Imaging Library (CIL), was proposed at the CCPi flagship pre-launch meeting at Diamond synchrotron. CIL will be the first complete CT analysis toolbox from CCPi for material imaging. Its first public release is scheduled to be 30 June 2017 with the majority of the codes in open source Apache 2.0 licence (some in dual licence arrangement).

Beam hardening code (part of CIL): The beam hardening correction software corrects the image data by estimating the polychromatic nature the X-rays used in lab based CT machines. This improves the quality of the downstream image reconstruction. In practice this technique is relevant to all lab based CT machines, which are prevalent in university imaging facilities in the UK and worldwide. The implementation is coupled with the image capturing process as part of the experiment setup, thus allowing correction of beam hardening effect prior to the application of the reconstruction algorithms. A version of this code has been released for user testing at Manchester X-Ray Imaging Facility (MXIF) at Harwell before the public release. This work was in collaboration with Graham Davis from QMUL, Matt Pankhurst, Loic Courtois, Peter Lee and others from the University of Manchester. Users have tested the code with the real experimental datasets and results are now being written up as a paper for Elseviser's Software-X journal (to be submitted in the next reporting period). The other major work undertaken for this code was to remove the dependency on the commercial Spekcal utility which generates an energy dependent spectra values from a tungsten source at a given angle. The significance of this is that our codes will be released as open source, allowing algorithm developers to improve our codes and users to test the software in other imaging facilities and instrument settings.

Reconstruction and ring artefact removal codes (part of CIL): The majority (7/12) CCPi codes use Matlab. Whilst Matlab allows rapid method and algorithm development and testing by mathematicians and method developers, it requires expensive Matlab licences and annual subscription, especially when specialist libraries, e.g. image processing toolbox, are used. This prevents our community to

test, adopt, and contribute to the code base. As a result, CIL, which includes reconstruction algorithms, e.g. CGLS, SIRT, and a ring artefact removal algorithm (Dr Valeriy Titarenko, Manchester University) have been packaged in Python language to improve its usability and accessibility. This opens up a wide range of possibilities for users to experiment our codes, methods, and analysis pipelines as they are based on freely available software and can be freely packaged and offered by any imaging facilities. The core team is actively prompting the adoption and exploitation of CIL in Harwell for the large facilities and in the university mid-range lab facilities. These codes are now included in SAVU (Diamond data analysis pipeline software), available to all Diamond imaging experiments in both physical and life sciences space along with the newly opened the Electron Bio-Imaging Centre (eBIC) at Harwell.

CIL Code distribution: A dedicated CCPi software distribution channel for CIL Python bindings is now created and this will enable easy installation of our software. For example, the latest version of SAVU is using this distribution channel for CCPi plugins.

The CCPi flagship proposal "A Reconstruction Toolkit for Multichannel CT" was awarded and it is going to build on top of the CCPi Core Image Library (CIL). http://gow.epsrc.ac.uk/NGBOViewGrant.aspx?GrantRef=EP/P02226X/1. This toolkit, when completed, will enable faster analysis of multichannel CT experiments. It aims to improve the segmentation of the reconstructed data and increases the accuracy of the experiment.

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

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

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.

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**

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 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. The 1.16 FTEs of the core support 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 imaging software. This includes 0.2 FTE for maintaining network, website, community support, running workshops and training courses and benchmarking, and 0.9 FTE for software engineering effort that contributes to SIRF development, testing, deployment and documentation.

CCP-PetMR – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

As well as administrative support for the CCP (organization of working group meetings, maintenance of web sites), the core support team will assist in:

- Standardise input and output data formats;
- Standardise software coding rules and testing;
- Assist with porting, parallelisation and optimisation on different hardware platforms including novel architecture systems.
- Provide centralised distribution and controlled releases for software;
- Provide installation user support for software, and run workshops/training events;
- Collate and distribute existing algorithms and code, including licensing requests;
- Encourage CCPs participants to make their algorithms and code available;
- Create a gallery of test real image and volume datasets for mathematicians to test and benchmark new algorithms; and
- Maintain documentation.

CCPPET-MR	Milestone	Target Date
	Website, mailing lists, source code and data archives *Task ongoing: the committee like the new website. Data archiving is being considered next.*	Ongoing
	Organise working group meeting, developers days and other event sessions *Task ongoing: Developers days are held every six weeks with around twenty attendees.*	Ongoing
	Support current training courses and organise developer workshop to teach *Task ongoing*	Ongoing
	Populate database for both simulated and acquired data (i.e. framework, will slowly be filled over the project) *Task ongoing: phantom data sets added. Now have first images.*	Ongoing

	Visit sites in the network to gain experience with a few selected packages for image reconstruction. Embedding within the main groups STiR and Gadgetron *Task ongoing: this is working well with Evgueni embedded at UCL every Thursday and Friday, and has also been to Manchester.*	Ongoing – embedding one day a week
	STiR code – API release (MATLAB or python) *Task complete: in MATLAB and Python*	Q1 2017
	Gadgetron code – API release (MATLAB or python) *Task complete: in MATLAB and Python*	Q1 2017
	Optional: STiR and Gadgetron combined release *Task complete: the official release will be Q2 2017 (12 May) but the software was complete in Q1 2017.*	Q2 2017
	Optional: Profiling and (if necessary speed-up) of 1 PET and 1 MR image reconstruction package *Task complete: used systems in SESC but have also built their own server. Conducted continuous integration testing via CCPForge. Achieved speed up of STiR under Windows of x1.5 faster*	Q1 2017
	Optional: Creation and maintenance of test-cases of PET/MR data and reconstructions – new release Q1 2017 *Task complete.*	Q1 2017

Staffing	**Effort**
Martin Turner	0.10 FTE
Evgueni Ovtchinnikov	1.00 FTE
New Hire	0.15 FTE
Erica Yang	0.05 FTE
Total	**1.30 FTE**

CCP-PetMR – Summary Report (1 April 2016 – 31 March 2017)

In the current reporting period, efforts have been primarily provided by Evgueni Ovtchinnikov and Ron Fowler. Approximately 0.5 FTE effort has been re-profiled to 17/18 and 18/19 FYs to accommodate a new recruit – Dr Eduardo Pasca who has started working on the project from April 2017.

Our work during the reported period progressed according to the job plan: software development and engineering efforts aiming for the first SIRF release, adding content for the website (www.ccppetmr.ac.uk); maintaining mailing lists (we now have 88 members on the CCP-PETMR announcement list – 6 new members joined since Nov. 2016, 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.

Our CCP Flagship proposal "A framework for efficient synergistic spatiotemporal reconstruction of PET-MR dynamic data" was awarded the EPSRC grant EP/P022200/1. This project, starting from 25 June 2017 for 32 months, will fund a full-time postdoc at UCL and part-time effort at STFC (28% Senior Software Engineer and 6% Software Engineer for software management).

Our open source software suite SIRF is on course for its first public release on 12 May 2017 (Release 0.9). This release is based on PET reconstruction package STIR (Software for Tomographic Image Reconstruction) and MR reconstruction package Gadgetron. 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. These are available on public CCP website.

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, 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 reduce the time required to test and validate PET-MR methods and algorithms before releasing the software publically.

Integrated help and user guides, as well as links to the OneDrive and Drupal archives are in continual development.

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

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

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.

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

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

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:

- TK organising the CCPBioSim/CCP5 "2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems, 13th-15th April 2016, Manchester (with Richard Henchman from CCPBioSim and Paola Carbone from CCP5)
- HL participating in the CCPBioSim training workshop in Bristol, June 8th, 2016: prepare tutorials and presentation for FESetup.
- Help with organising training workshops, at an expected level of 3 per year. This usually involves handling the registrations and any associated fees, though additional help can be given to the local organisers as needed.
- Help with organising the CCPN joint conference in July in Buxton lead by Julien Michel.
- TK to organize a CCPBioSim ChemShell QM/MM training workshop at Daresbury in early 2017.
- Help organise joint experimental-computational workshops, at an expected level of 1 per year.
- Help Simone Breckell (admin support for CCPBioSim at Bristol) with organisation of industry 'sandpits'. A link to the Hartree Centre may be useful here.
- Maintain the website http://www.ccpbiosim.ac.uk on the new server at Daresbury.
- Manage email list ccpbiosim@jiscmail.ac.uk
- Support use of 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:
FESetup will see further enhancements to its functionality. A particular request from the user community is to support side–chain mutations for proteins (generally: mutations of covalently linked residues in a polymer). The code should also support other free energy simulation methods like Umbrella Sampling. Software support is currently mainly focused on the development of FESetup. Additional software projects should be looked into to sharpen the profile of CCPBioSim and widen support to more users, e.g. the GLAS GCPR scoring code.

Work planned for this period:

- Prepare for the workshop in Bristol June 8th, 2016: prepare tutorials and presentation
- Implement a new data format to package setup files and associated data and descriptors created through FESetup.
- Release FESetup 1.2 by May 31st, 2016: user improvements like simpler path lambda selection (choice of vdW from electrostatic lambda separation), choice of ionic strength, consistent output file naming; full support for all protocols for pmemd/sander, Gromacs and Sire, absolute transformation for Sire, use the new data format for restarts, base on AmberTools 16 and Propka 3.1, support GAFF2
- Add support for arbitrary mutations of covalently linked residues in a polymer. Plan is to use the same flexible MCS approach as currently used for ligand setup.
- Better support for binding mode preservation.
- Integrate with Lomap2 to automate morph pair selection and better control over MCS selection.

- Finish the Reproducibility study carried out in collaboration with Julien Michel (Edinburgh), David Mobley (UC Irvine), Benoit Roux(Chicago)) and publish results.
- Implement support for ProtoMS. This will be needed for the Free Energy Workshop in autumn in Southampton. FESetup will be presented and used for the setup of the tutorials. Help in organising the workshop.
- In addition to virtual machine images, provide Docker images. This will be useful for demonstration purposes e.g. to industry and ensure that FESetup can run with easy installation on unsupported platforms.
- Integrate Longbow into FESetup to enable off-loading of computationally expensive setup steps to remote HPC resources.
- Add support for umbrella sampling within FESetup. This will later be extended to string-type methods (with Edina Rosta, KCL) possibly implemented in Plumed (with Francesco Gervasio, UCL).
- Look into support for LAMMPS and if there is sufficient interest.
- Implement the new OPLS-AA/M force field into FESetup and see how to extend this to general ligands.
- Start implementing the GLAS GCPR scoring code

CCPBioSim	Milestone	Target Date
	Successful completion of multiscale modelling conference *Task complete: The conference was held at the Manchester Conference Centre, April 13-15 2016, featuring 21 speakers from around the world and was sold out with over 90 attendees*.	Q2 2016
	Release of FESetup 1.2 *Task complete: FESetup 1.2 was released in May as planned , supporting perturbed topology files for a wide range of simulation software packages.*	Q2 2016
	ProtoMS support and Free Energy Workshop *Task in progress: ProtoMS support under development, targeting 2017/18 for completion*	Q2 2017
	Integration of FESetup with Longbow (HECBioSim) *Task in progress: Integration work ongoing; completion expected in 2017/2018*	Q2 2017
	Support for side chain mutations (FESetup 2.0) *Task in progress: Currently evaluating two different approaches to supporting this, aiming for completion in 2017/18. This code will be released as v2.0.*	TBC 2017/18
	~~Release of FESetup 2.0~~ *Task combined with previous task*	~~Q4 2016~~
	Reproducibility study *Task complete: Study aimed at answering whether alchemical free energies can be reproduced with AMBER/Gromacs/CHARMM/OpenMM is now complete and a manuscript is in preparation*	Q1 2017
	Support for umbrella sampling within FESetup *Task ongoing: this task may no longer be required. Currently consulting the community to investigate whether there is a need for this development*	Q1 2017
	Organise a free energy workshop including FESetup *Task complete: An FESetup workshop was held as part of the BioSim tutorial workshop week in Bristol in June*	Q4 2016

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

CCP-BioSim – Summary Report (1 April 2016 – 31 March 2017)

The project has proceeded as planned with Hannes Loeffler working full time on SLA activities. In April Tom Keal took over from Martyn Winn as SLA lead for STFC, responsible for coordination of SLA effort with the CCPBioSim management group and networking activities.

The main focus of software development in CCPBioSim is FESetup, a program developed by Hannes Loeffler which makes biomolecular calculations more accessible to the community by automating the setup of input files for molecular dynamics simulations and protein-ligand free energy (FE) calculations. Version 1.2 was released in May, greatly simplifying the creation of inputs for a wide range of simulation software packages: AMBER, Gromacs, CHARMM and Sire. Support for the ProtoMS code (Jonathan Essex, Southampton) is currently under development, which would enable free energy calculations using Monte Carlo methods. To make the code easier for users to run on any operating system a virtual machine image has been produced and a new data file format has been introduced which makes packaging and distribution of simulation setups easier and more consistent.

A reproducibility study carried out by Hannes Loeffler aimed at answering whether alchemical free energies can be (within statistics and simulation protocol) reproduced with the programs AMBER, Gromacs, CHARMM and Sire/OpenMM is coming to a close and a manuscript is now being compiled. This type of benchmarking is important to assure that users can obtain reliable results across codes. It will also be a crucial test for FESetup to demonstrate that the code is fully capable of generating inputs for all supported MD packages.

The 2nd joint CCP5/CCPBioSim Multiscale Modelling Conference was held at Manchester Conference Centre, 13-15th April, bringing together the biological and materials modelling communities to discuss topics of common interest. Tom Keal lead the organisation together with Paola Carbone (CCP5) and Richard Henchman (CCPBioSim). 95 researchers attended to discuss topics across the spectrum of electronic structure, atomistic and mesoscopic scales and to address the current and future challenges posed by multiscale modelling.

Hannes Loeffler and Tom Keal also represented CCPBioSim at another joint event, the “Simulations for the Experimentalist and Industrialist” workshop held at Diamond Light Source, where they gave presentations on biomolecular modelling aimed at non-specialists.

A CCPBioSim tutorial workshop week was held at Bristol 6th-10th June organised by Marc Van der Kamp with contributions from Kara Ranaghan, Christopher Woods, James Gebbie, Charles Laughton, Hannes Loeffler and Adrian Mulholland, covering enzyme-ligand modelling, MD simulations, Python for Biomodellers and FESetup, Monte Carlo methods and QM/MM modelling.

A 4-day CCP5 Summer School was held at Lancaster 11-19 July. Richard Henchman and Syma Khalid contributed to this: they organised and delivered an Advanced Course on Simulation on Biomolecules which focused on demonstrating how the concepts and principles already taught in the main course can be applied to simulate biological molecules as well as providing a discussion of some of the state-of-the-art methods for simulation of biological molecules. 30 students out of 70-80 attended this optional module.

A 4-day CCPN/CCPBioSim joint conference was organised by Julien Michel at the University of Derby in Buxton, 25-28thJuly, covering new methods and applications of biomolecular simulations,

biomolecular NMR, and the interface between computation and experiments. The meeting attracted 123 delegates from the UK and across the EU. There were a total of 20 invited speakers and 34 poster presentations. 8 of the invited speakers had been nominated by CCP-BioSim. The other 12 speakers included scientists with expertise in NMR and other biophysical methods, and scientists with dual expertise in simulations/NMR.

An AMOEBA advanced potential energies workshop was held on 9 December 2016 at Southampton lead by Richard Bradshaw, Frank Longford, Noor Mohamed and Jonathan Essex.

Atomistic Simulation of Biocatalysts for Non-Experts was held in Manchester on 23 February 2017, organised by Marc van der Kamp in association with the UK Catalysis Hub.

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

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

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.

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

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Embedded cluster and Quantum Mechanical methods

The ChemShell code for QM/MM calculations is currently in transition from a Tcl-based code (v3) to a Python-based code (v4). In the support period 2016-2017 we expect to release a beta version of ChemShell v4 for testing, but the Tcl-based ChemShell will remain the official stable version, e.g. as a module on ARCHER. Python-ChemShell is being developed in close collaboration with MCC academic groups, and it is appropriate to use MCC effort to develop extra features in Python-ChemShell in preparation for its final release. The milestones this year therefore again contain both Tcl-ChemShell and Python-ChemShell tasks:

- Integration of GULP QM/MM-compatible force field setup scripts into Tcl-ChemShell distribution and Python-ChemShell to simplify setup of the embedded cluster model for general users.
- Development of a ChemShell extension in the STFC-developed visualiser Aten to support setup of embedded cluster QM/MM calculations (e.g. ChemShell file format support, selection of regions)
- Extension of (LS)DALTON interface in Python-ChemShell to directly link Dalton in as a library for increased efficiency on HPC platforms, following the scheme used in Tcl-ChemShell

DL_POLY development and support

Development and application of classical statics and dynamics particle based code. Support and training to DL_POLY and DL_FIELD users from MCC. Dissemination of new developments in DL_POLY and their application, impact via publications and presentations at national and international conferences.

DL_POLY_4 provides access to particle dynamics techniques; MS, MD, DPD with a range of user tools implemented as optional functionalities. DL_FIELD (DL_ANALYZER) is a facilitator programme that provides access to system models used to in the design and build up of bio-chemical, organic and generally soft-matter materials systems by producing the necessary input files needed for DL_POLY, DL_MONTE and DL_MESO. It also provides functionality aimed at solid state materials and can be used to design and build up organic-inorganic interfaces. DL_POLY is widely used by the MCC consortium whereas DL_FIELD is yet to make a larger impact. It is thus appropriate to assign some MCC effort to expose the package capabilities to the consortium via training and 1-2-1 coaching where needed as well as enhance and develop extra features of most use to users. The milestones for this year for DL_POLY and DL_FIELD are as follows:

- Organisation of presentations at MCC meetings and specific workshop where both DL_POLY and DL_FIELD are showcased. Q3 2016/Q1 2017
- Development of a workflow that demonstrates the use of DL_FIELD in the design and production of organic inorganic interface system, which is then run by DL_POLY. Q3 2016
- HPC effort to improve the performance of the recently released multipolar electrostatics developments in DL_POLY. Q2/3 2016
- Contribution to collaborative effort (Henry Boateng, Bates; Ian Bush, Oxford) to investigate the inclusion of electric field calculation and consecutively the implementation of instantaneous dipole polarisability schemes for multipolar electrostatics. Q2 2016/Q1 2017
- DL_FIELD provide a standardised inorganic force field library to facilitate both construction and selection of inorganic field force models. Similar to organic force fields, a standardise atom typesetting system is to be implemented so as to smoothen implementation of bio-inorganic systems. Q1 2017

CRYSTAL development and support

Development and application of the CRYSTAL code to the study of excited states and dynamics in extended systems. Work on *ab initio* modelling of catalytic processes. Support to CRYSTAL users from MCC and other UK communities (including STFC Facilities users). Training of CRYSTAL users. Dissemination of new developments in the code and their application in publications and at national and international conferences.

	Milestone	**Target Date**
MCC	**ChemShell/DL-FIND**	
ChemShell	Integration of GULP force field setup scripts into ChemShell (TWK) *Task complete*	Q2 2016
	Directly-link (LS)DALTON into Python-ChemShell (TWK) *Task complete: fully functional for QM/MM calculations including with shell model forcefields.*	Q1 2017
	ChemShell support in Aten (TWK) *Task complete. Support for the ChemShell file format is in the Aten repository.*	Q1 2017
	Support for ChemShell and GAMESS-UK on ARCHER (TWK) *Task continues on an ongoing basis. ARCHER support is up-to-date. Also installed ChemShell on the Cardiff RAVEN cluster and Bristol BlueCrystal phase 3 for use by academics there..*	Ongoing
DL_POLY/ DL_FIELD	Organisation of presentations at MCC meetings and specific workshop where both DL_POLY and DL_FIELD are showcased. *Task in progress: material and staff preparation completed. Waiting for dates to be fixed.*	Q1 2017
	HPC effort to improve the performance of the recently released	Q3 2016

	multipolar electrostatics developments in DL_POLY. *Task in progress: good progress has been made. Completion may move to Q1 2017 due to some of the effort being redirected towards grant preparation and staff supervision.*	
	DL_FIELD provide a standardised inorganic force field library to facilitate both construction and selection of inorganic field force models. Similar to organic force fields, a standardise atom typesetting system is to be implemented so as to smoothen implementation of bio-inorganic systems. *Task in progress and on target.*	Q1 2017
	Support for DL_POLY_4 on ARCHER (ITT). Support for DL_FIELD (CY) *Task in progress and on target.*	Ongoing
CRYSTAL	Supervision of work on (photo-induced) dynamics of molecules in solution in collaboration with ISIS and CLF. – Initial set up of at least one system and feasibility study. *Task complete*	Q2 2016
	Supervision of work on curing pseudo-linear dependence in CRYSTAL calculations (MCC/eCSE project) – Demonstrate improvements in the overlap matrix calculation using metallic Na as a test case. *Task complete: report submitted to eCSE panel.*	Q3 2016
	CRYSTAL simulation of excess electron states in solid and liquid methane – In collaboration with Prof N Quirke, Imperial College London *Task complete*: *paper published September 2016.*	Q3 2016
	Preparation of lectures and attendance at CCP5 Summer School on molecular simulation *Task complete*	Q2 2016
	Preparation of lectures and attendance at MSSC2016 CRYSTAL Summer School *Task complete*	Q3 2016
	Improvement of TD-DFT routines in CRYSTAL, in collaboration with Turin CRYSTAL developer groups. Extension of matrix formalism (generalised Casida's equation) to full **k**-dependence and tests for molecules, polymers, surfaces and three-dimensional crystals. *Task complete: This project has been expanded considerably, in order to make the code more general and robust. A set of test cases for the new functionality are available.*	Q4 2016
	Development of formalism (plus possibly test implementation) of CP generalised Lagrangian density matrix propagation scheme for MD in CRYSTAL. *Task complete: The GLDM propagation scheme for MD in CRYSTAL has been discussed with collaborators in Turin and Oxford. A preliminary implementation of the DM propagation has been coded in the current version of CRYSTAL14, although further work will be required to have a generally usable code.*	Q4 2016
	General support to CRYSTAL users *Task ongoing.*	Ongoing
	LB to visit Turin CRYSTAL developer group for update about UK CRYSTAL developments, discussion on TD-DFT and MD	Q2 2016

	developments and general plans about UK code integration into official code release in Italy. *Task complete: one more visit took place in October.*	
	Paper on multiferroic GaFeO3 – in collaboration with Nic Harrison and Robert Cernik *Task in progress.*	Q1 2017
	Paper on dynamics of molecules in solution – in collaboration with T. Parker and R. Bisby *Task in progress.*	Q1 2017

Staffing	**Effort**
Leonardo Bernasconi	1.00 FTE
Barbara Montanari	0.25 FTE
Iilian Todorov	0.60 FTE
Chin Yong	0.15 FTE
Tom Keal	0.50 FTE
Total	**2.50 FTE**

MCC – Summary Report (1 April 2016 – 31 March 2017)

CRYSTAL (1.25FTE): CRYSTAL is one of the leading codes worldwide for the calculation of structural, electronic and optical properties of solid-state systems, and it has been under continuous development for almost 40 years at STFC in collaboration with the University of Turin (Italy). CRYSTAL is an important component in the landscape of first principles electronic structure codes because it is the only code conceived from the beginning to use Gaussian basis functions for representing the electronic states in periodic systems. This in turn makes it possible to deploy powerful screening techniques to exploit real space locality, leading to a better scaling of the computational cost as the system size increases.

The main aim of the project supported by MCC (1.25 FTEs) is to develop new functionalities in the ab initio electronic structure software CRYSTAL, to test and optimise the code for usage on large UK supercomputers (including Archer) and to provide training and one-to-one support to new and existing users. The project lead is also responsible for directing the community of UK developers of CRYSTAL, which includes senior researchers at STFC (RAL and DL), Oxford University and Imperial College London, and to facilitate the interaction of the UK developers with the core developer group at the University of Turin (Italy), led by Professor Roberto Dovesi.

The code developers are involved in several scientific projects with UK and international universities, MCC members and with major UK experimental Facility users (the ISIS Neutron and Muon Source, the STFC Central Laser Facility and the Diamond Light Source). Although CRYSTAL is the main software used in these projects, other ab initio codes well known to MCC users are also frequently employed, and informal support is provided to users.

The main technical focus of the project is currently on the development of new methods for the treatment of excited states in extended systems in CRYSTAL. This is an important step for the accurate and reliable prediction of spectroscopic properties (e.g. UV-vis and fluorescence) of solid-state materials and complex molecular assemblies, with potential impact in photo-voltaics, photo-catalysis and in the study of radiation damage in materials. We also work on ab initio molecular dynamics techniques (particularly in the field of homogeneous catalysis) and on the extension of the CRYSTAL code to the treatment of large (1000-10000 atoms per cell) systems.

The most important technical aspect that we have considered this year has been the proper treatment of quantum-mechanical exchange interactions in the time-dependent DFT approach for the

calculation of excited states in solids, which was implemented by Leonardo Bernasconi in the CRYSTAL code in previous years. In previous work, we have shown that the standard treatment of exchange in CRYSTAL is sufficient to describe low-lying excited states (e.g. excitons in semiconductors) accurately, but fails for higher energy states. This renders the description of, for instance, X-ray based spectroscopies virtually impossible. There is at present no software capable of treating exchange properly and efficiently for high-energy excited states in infinite periodic systems and, if successful, this development will make CRYSTAL a powerful and unique tool to study the response of wide classes of materials to radiation of any wavelength. Coupled with the superior scaling with system size exhibited by the massively-parallel (MPP) version of CRYSTAL, this work will pave the way for the study of new materials and their response to radiation, a long sought after goal in materials discovery and photo-voltaics.

We have also worked at an important technical extension of CRYSTAL to treat with improved accuracy systems requiring large and diffuse Gaussian basis sets, like metals or crystals in unusually close packed geometries. This work has been supported through and Embedded CSE (eCSE) grant involving STFC (Leonardo Bernasconi and Dr Barry Searle at DL) and MCC members at Imperial College. The work is complete and a full report is available on the Archer website.

A number of collaborative scientific projects have been carried forward during the reporting period concerning the simulation of excited states in disordered polymers (Chem. Phys. Lett. 664, 143 (2016)), of oxidation catalysis in solution using ab initio molecular dynamics (ACS Catalysis, submitted) and of laser induced structural transformation in new anticancer drugs (in collaboration with the STFC Central Laser Facility).

DL_POLY (0.61FTE): The DL_POLY project is the jewel in the crown of STFC's in-house developed computational projects. DL_POLY_4 is the current UK flagship package for classical molecular dynamics, led and developed by its principal author Ilian Todorov. The size and functional complexity of DL_POLY_4 is so large that any complexity step-change work can only be achieved by joined SLA/COSEC effort with CCP5 and further complementary support via EPSRC, NSF and d/eCSE software capability funding schemes. Training and HPC methodology prototyping are also supplemented by other small effort streams coming from Intel Parallel Computing Centre funding, Energy Materials Computational Solutions consortium and last but not least PRACE.

The DL_POLY project recruited two new members Vlad Sokhan (January 2016) and Ivan Scivetti (March 2016) to implement shaped particle dynamics and empirical valence bond functionality in accordance with effort levels and plans of CCP5 SLA/COSEC. Projects' supervision and management are provided by Ilian Todorov and Alin Elena.

The DL_POLY GitLab repository has been extensively improved with code peer-review processes and enabling action and comments response by email. These practices are established in assistance with Alin Elena and enforced to ensure code quality regulation and thus long-term software sustainability.

Recent developments include CHARMM model enablement for self-induced polarisation of intra-molecular interactions, improved core-shell filtering, new "zero K fire" optimisation option, "zero K stress" calculation, etc. The optimisation options have been used in assisting collaborative research in MCC relevant projects led by Prof. Richard Catlow (UCL), Prof. Nora de Leeuw (Cardiff) and Prof. Martin Dove and Dr. Kostya Trachenko (QMUL). The improved core-shell filtering simplifies procedures for selecting core-shell polarisation units in a number of places of the code where the functionality affects the calculation of various force-flied components and during integration. This improves the performance for models with many polarisable species as well as when systems' intra-molecular complexity (topology and chemical description) dominates over the inter-molecular one.

The CHARMM model enablement open the doors to using CHARMM models for many bio-chemical and organic systems expanding the appeal of DL_POLY to communities beyond MCC and CCP5 such as CCPBioSim. The implementation also enables inexperience users to set up core-shell interaction parameters in an automated manner by providing only atomic polarisation. The optimisation and "zero K fire" options work provides a more enhanced pathway to energy minimisation procedures which has proved to be problem for setting up and equilibrating initial system design for mixed organic/inorganic models with challenging complexity such as zeolite frameworks, pure organic frameworks and metal-organic frameworks. It also decouples the minimisation stepping from atomic clock stepping and thus facilitate systems with disparate clocks such as ones with both atomistic and coarse-grained subsystems. Zero K stress calculations enable DL_POLY being used in meta workflow packages for generation of atomistic potentials via global minimisation of DFT runs in packages such as MEAMFIT (by Andrew Duff).

The CHARMM functionality is awaiting for scientific testing and assistance from Dr. Henry Boateng at Bates College (USA), who together with Ilian Todorov is also involved in collaboration with Prof. Graeme Day (Southampton) in enabling DL_POLY_4 as substitute of DL_MULI for modelling of Porous Organic Molecular Crystals using multipolar electrostatics.

DL_FIELD (0.14FTE): DL_FIELD is a user-friendly force-field facilitator toolbox for the DL_POLY, DL_MESO and DL_MONTE projects. Authored by Chin Yong, it is designed to handle molecular information with minimum user's intervention and effectively create, convert, transform and extend force-field models for the most popular codes in the CCP5 library. Complementary to its editing abilities, DL_FIELD also develops its own notation nomenclature, DL_F, which caters for the automatic identification of chemical nature of every atom in a system and description of consistent atom typing for a range of FF schemes.

Major reorganisation of the program structure was carried out in preparation for implementing the multiple potential model setup capability. This enabled the setting up of force field models that consist of a number of different force field schemes including inorganic and organic force fields. The feature was made available in the version 4.1 released in December 2016. In addition, preliminary work had started to reorganise the inorganic force field library and classify force field models according to types of materials.

CHEMSHELL: The ChemShell computational chemistry environment is currently being redeveloped as a python-based programme. This now has a fully functional implementation of a driver for combined quantum mechanical and molecular mechanical (QM/MM) calculations, which is suitable for solid state modelling of complex systems using the QM codes NWChem/GAMESS-UK and the MM code GULP. This code is being extensively tested on example systems provided by MCC users. MCC support has accelerated development of the software through features of specific interest to the consortium and of relevance to ARCHER such as a new MPI parallelisation framework, and the code is continuously tested on ARCHER as it is developed. We are targeting Q3 2017 for an initial beta release of Python-ChemShell to the community. MCC support is also vital for the continued support of the current Tcl-based version of ChemShell, which is the release currently available to users on ARCHER. We continue to maintain ChemShell and GAMESS-UK on this platform and have also installed it on the RAVEN cluster for MCC users at Cardiff.

Tom Keal gave a talk on recent developments in the ChemShell and DL_FIELD packages at the Materials Chemistry Consortium meeting on 21 December 2016.

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

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

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.

Staffing	Effort
Leonardo Bernasconi	1.00 FTE

~~Barbara Montanari~~ Barry Searle	~~0.25~~ 0.22 FTE
Ilian Todorov	0.75 FTE
Tom Keal	0.50 FTE
Total	**~~2.50~~ 2.47 FTE**

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

The activities below will be carried out by Dominik Jochym thanks to the 1FTE funding for core support. In addition, Peter Byrne (Durham University) will be providing software development support amounting to 0.42FTE due to DBJ's sickness leave.

UKCP	Milestone	Target Date
	Investigate viability of transfer of CASTEP's continuous integration from Builedbot to Jenkins *Task complete: this will be put into production in 2017.*	Q2 2016
	Co-organization and teaching of CASTEP workshop in Oxford = 1 month *Task complete: workshop went well with sixty six attendees*	Q3 2016
	Finish implementation of "2n+1" Raman and NLO code in CASTEP *Task complete: now included in the CASTEP repository. Task was completed on time and has been released as DFPT Raman.*	Q4 2016
	Release management of CASTEP v17.2 including documentation and liaison with major HPC services *Task complete: delayed due to leave but went ahead in Q1 2017..*	Q4 2016
	Extend polarisation (Berry phase) code to include USPs *Task removed: this work is being completed outside STFC and is being overseen by Hasnip (York) and Yates (Oxford).*	Q2 2017
	Organisation of 2017 CASTEP "codefest" core developer workshop *Task complete: the event was a resounding success and was considerably more productive than previous codefests.*	Q2 2017

Staffing	Effort
Dominik Jochym	1.00 FTE
Peter Byrne (Durham)	0.42 FTE
Total	**1.42 FTE**

Peter Byrne (Durham University) is funded from STFC for 6 months from 1 March 2016 to deliver the effort that was not delivered in 2015/16 due to staff illness**.**

UKCP – Summary Report (1 April 2016 – 31 March 2017)

Effort has primarily been provided by Dominik Jochym. Peter Byrne (Durham University) provided six months of work to make up for a reduction of effort during 2015/16 due to staff illness.

Raman spectroscopy is widely used to obtain information on the chemical composition and structure of compounds across the physical and biological sciences. The ability to compute Raman spectra from first principles provides an invaluable tool to interpret experiment and to gain insight into the relationship between structure/composition and experimental observables. Peter Byrne has helped to complete Dominik's work on the Density Functional Perturbation Theory (DFPT) Raman code in CASTEP, and under Dominik's guidance, has prepared this for the upcoming CASTEP v17.2 release. This newly completed functionality will replace a previous implementation of Raman intensities with code that is not only faster but also scales better with system size. To date, Raman calculations with CASTEP have been limited to fewer than 100 atoms and have been relatively niche in application. This new development will move Raman calculations into routine use for the analysis of vibrational spectroscopy for systems of size up to ~1000 atoms.

The academic source code of CASTEP v17.2 was released at the end of February 2017. In addition to the above mentioned new DFPT Raman functionality, this release includes several "quality-of-life" changes for users to carry out simulations more efficiently and with better accuracy "out-of-the-box".

Continuous integration (CI) is an important part of the maintenance and quality of large software development projects. 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 CASTEP project has made successful use of the Buildbot CI system for some years, however the service is not actively maintained so an alternative is required. A viability study into the benefits of a migration to the Jenkins continuous integration service hosted on CCPForge (supported by SESC) has been conducted. After a successful pilot test, the Jenkins system will be adopted by the CASTEP project. That the service is integrated with CCPForge has the benefit of accessibility for existing CASTEP developers and users and sets a path for larger community code development contributions in the future.

In August, UKCP and CCP-NC joined forces to hold a CASTEP workshop in Oxford, and Dominik Jochym helped with the organisation of the event as well as the delivery of the training material. The highly successful event was at full capacity with 66 participants – discussions are ongoing to move to a larger venue for the lectures to allow up to 100 delegates from 2017 onwards. Of this year's participants, 48 were primarily experimental scientists. This demonstrates the continued upward trend of computer simulation's adoption into experimental workflows.

Dominik Jochym also assisted with the organisation of the 2017 CASTEP "Codefest" core developer workshop. During this week-long, yearly event, all major CASTEP developers come together to push forward the development of the code and discuss scientific and strategic topics.

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

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

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 developers 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.

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

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 focused 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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

SLA support for UK-COMES will focus on the on-going development of the DL_MESO Lattice Boltzmann (LBE) module as a community code for engineering applications.

The coming year will see a variety of specific items of LBE functionality added to DL_MESO, including a number which have already been implemented elsewhere but which will be brought together and supported within DL_MESO for the use of the community. Decisions on implementions for applications and their timings based on collaborations with other consortium members will be agreed upon during the year.

Other more generic functionality developments during the year are expected to include:

- Solid/fluid interactions (Ladd algorithm)
- Fluid-filled vesicles based on Lishchuk continuum-based multiple fluid algorithm
- Implementation of the Large Eddy Simulation model for turbulent flows
- Immersed boundary method for deformable solid boundaries

The use of the OPS framework to implement LBE simulations on multiple computing platforms (including GPU and accelerators) for non-cuboidal systems with a finite difference solver for turbulence models will be explored. Work will also be carried out in collaboration with (and funded by) Intel to produce a port of the DL_MESO LBE module for Intel Xeon Phi systems.

UKComes	Milestone	Target Date
	Implementation of solid/fluid interactions *Task in progress: will be completed during Q2 2017*	Q2 2016
	Testing of OPS with DL_MESO *Task in progress: testing is underway. A proposal was submitted to the software for the future call that will make use of OPS. This project has now been funded with £0.5m and will start in June 2017. Jianping Meng is the PI and Michael Seaton is one of four Co-I's. Jianping has been testing and is almost done but the task will roll over into next year's plan as a consequence of the funding.*	Q3 2016
	Implementation of fluid-filled vesicles *Task ongoing: this task may slip as agreed with head of UK-COMES due to other workload. The collaborator at Sheffield Hallam has funding for a PhD who will take this task on. Michael will be an external supervisor. Will move into 2017/18.*	Q1 2017
	Implementation of Large Eddy Simulation turbulence model *Task ongoing: this task may slip as agreed with head of UK-COMES due to other workload.*	Q1 2017
	Implementation of immersed boundary method *Task ongoing: Jianping not started yet. OPS work took priority. This task has changed slightly and will be covered by the OPS task in 2017/18.*	Q1 2017

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

UK-COMES – Summary Report (1 April 2016 – 31 March 2017)

Work has progressed smoothly. Plans were changes slightly, in agreement with the community, to accommodate the preparation of a proposal for an EPSRC Software Flagship Project Call in August/September 2016, which was successful. One milestone (implementing solid/fluid interactions) is now due to be completed by the end of Q2 2017, while another (immersed boundary methods) has been carried over into 2017/18 for completion in Q3 2017.

Cascaded Lattice Boltzmann collisions allow LBE simulations of fluid flows at high Reynolds numbers (large velocities, low viscosities) and the capability of modelling turbulent flows, which are often found in industrial processes. Michael Seaton has added this model to DL_MESO's LBE code as an additional option for particle collisions, expanding on simpler but numerically less stable single and multiple relaxation time schemes. This functionality is currently undergoing testing ready for the next release of DL_MESO.

A two-dimensional version of DL_MESO's LBE code using the Oxford Parallel library for Structured-mesh solvers (OPS) has been successfully implemented 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 community. Tests for single fluid systems demonstrate good to excellent performance and scaling on both CPU and multiple-GPU based systems. A few more functionalities have been added to the code to improve its capability of modelling single-fluid systems (see the list in the table below) and testing is ongoing.

Based on the above work with OPS, a proposal was prepared and submitted (led by Jianping Meng) on behalf of UKCOMES for the EPSRC Software Flagship Project Call to develop a high-level coding abstraction system: the High-Level Mesoscale Modelling System (HiLEMMS). This system will exploit the 'code once, compile and run anywhere' approach to automatically generate efficient LBE-based codes for multiple computing architectures and allow couplings to non-uniform grids and other grid-based modelling techniques (e.g. finite difference discretisation in physical space). HiLEMMS will be used as the basis of reengineering DL_MESO to allow efficient execution of LBE simulations on any given computing system and to tackle geometrically complex systems of both scientific and industrial interest. This bid was ultimately successful and three years' of funding is due to start from June 2017.

A UKCOMES workshop was held at University College London, specifically on Lattice Boltzmann methods and applications: Jianping Meng presented a talk on 'Discrete Boltzmann model of shallow water equations with polynomial equilibria' and acted as a section chair, and Michael Seaton gave a presentation on 'Modernisation of Lattice Boltzmann codes'.

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

(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 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..

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

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

Specific plans for this year are:

1. On-going maintenance of the HECBioSim portal, including updating information on applications for time, updating the HECtime calculator for new versions of MD codes, adding new software to the repository, etc.
2. On-going maintenance of the CCPBioSim portal. In particular, launch the Research Highlights pages.
3. As a new software project, work with the Essex group (Southampton) on the following modifications to LAMMPS:
   a) The implementation of the symplectic and time-reversible rigid body integrator developed by Dullweber, Leimkuhler and McLachlan (DLM) in the LAMMPS software. (Dullweber, A.; Leimkuhler, B.; McLachlan, R. J Chem Phys 1997, 107, 5840)
   b) The modification of the existing Parrinello Rahman constant pressure barostat to support the new integrator in the context of combined atomistic and rigid body molecular dynamics in LAMMPS.
   c) The combination and optimisation of rRESPA multiple-timestep algorithm with this integrator and barostat in the context of dual-resolution molecular dynamics simulations in LAMMPS.
   d) The modifications implemented in LAMMPS will be tested on a range of simulation systems of increasing complexity appropriate for determining the correctness and performance of the code.
4. GPCR-GLAS – Support CCPBioSim with the implementation of the GPCR GLAS scoring plug-in for Gromacs.
5. Longbow – Longbow is now in stable release, so the focus will be maintenance and inclusion of new features requested by the community. The following are already planned:
   a) Machine specific batch limits, user should be able to set the number of queue slots available for different queues and Longbow will simply batch the submit commands such that full automation can be achieved without violating queue policies or having complex arrays.
   b) Linking Longbow to the online calculator tool. This could have two routes; the first being that Longbow could simply take information from the calculator to further simplify the user experience in using Longbow. The other is that Longbow could collect metadata from user simulations and feed this information back to our sever for inclusion into the calculator, allowing us to improve the calculator accuracy and even support new codes we know nothing about!
   c) Support Hannes with the integration of Longbow into FESetup. This should be a similar case to supporting CCP-EM into the best practice of integrating Longbow.
6. Promote HECBioSim and Longbow at meetings, for example the CCPBioSim annual meeting in September 2016.

HECBioSim	Milestone	Target Date
	Launch the CCPBioSim / HECBioSim Research Highlights *Task in progress: waiting for contributions. This is more a support role to the individual groups. Progress is being made. Sarah Harris is in charge of gathering the information and she is currently generating the animations. The task has been moved onto next year's plan..*	Q3 2016
	At least one LAMMPS extension coded and deposited	Q4 2016

	Task complete: the community no longer have an appetite for this task and it was removed following discussion at the management group meeting on 16 December 2016.	
	Linking Longbow to the online calculator tool *Task complete: the prototype is being worked on by James Gebbie. This task is specific to ARCHER. It will use the benchmark tools and distribute them as a separate Longbow benchmarking system.*	Q1 2017
	GPCR-GLAS scoring plugin for Gromacs *Task complete: this task was abandoned as there was no longer any requirement for the work..*	Q4 2016

Extra time created by the abandoned tasks went on new releases of Longbow. There have been eight releases this year. Plus some work on the HECBioSim website around security audits.

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

HECBioSim – Summary Report (1 April 2016 – 31 March 2017)

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

James has begun work on benchmarking the latest versions of molecular dynamics codes (AMBER, GROMACS, LAMMPS, NAMD) on ARCHER and other computing platforms, in particular those with hardware accelerators such as GPU and Intel Xeon Phi. This activity 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. Work so far has focused on preparation of the benchmarking suite to ensure it is compatible with the latest codes.

Longbow is the light-weight HECBioSim simulation submission engine developed by James and part of a collaboration with Charlie Laughton (Nottingham). Longbow allows a user to launch simulations to High Performance Computing (HPC) machines in a manner that closely mimics how they already run them on their PC. Longbow handles all scheduling, monitoring and file transfer and is capable of doing complex multi-machine scheduling. Currently Longbow has been downloaded 4,857 times. Some of the key developments in this reporting period are:

- Implemented a Recovery mode – Should the event happen that Longbow crashes or the system in which Longbow is controlling jobs from powers down. The user can now reconnect to the crashed session and carry on as if nothing happened.
- Sub-Queuing – More and more system administrators are setting limits not just on the number of simulations that can run, but also on the number of jobs that can go into the queue. Longbow can now automatically detect this and implement its own queue feeding jobs into the system queue as slots open up.
- Dis-connectible/Re-connectible Longbow sessions – A user can now launch Longbow to fire off all jobs and then disconnect, at a later date the user can re-establish the connection and download all results (no need for persistent connections anymore)
- A concerted effort to introduce continous integration principles into the Longbow development process, this included writing more than 600 unit tests, a major code refactor and fixes for many bugs found during implementation of automated testing. A shift to this method of development will enable better collaborations for code development in the future.

- Ability to include scripts in the Longbow generated submit files.
- Numerous stability, performance and bug fixes

The uptake of Longbow into other projects has also increased in this reporting period. 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 currently working to include Longbow in their code base, one aimed at automated compilation, and runtime performance optimisation and tuning. The other a biosimulation setup, launch and analysis workflow tool.

James has updated the HECBioSim website and server to maintain a high level of security, and to keep the information current. The HECTime documentation has been improved by simplifying the language and reducing ambiguities.

HECBioSim was represented on the second day of the CCPBioSim Training Week with training in running and analysing MD simulations. This day introduced users new to biosimulation to how to set up a basic simulation (Chris Wood) through how to use Longbow to scale up to massive volume simulation (James Gebbie), and finally to how to analyse such large volumes of data (Charlie Laughton). There were 48 attendees.

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

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

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:
    1.1. 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.
    1.2. Collect data from the benchmark suite.
    1.3. Generate a predictive model based on the benchmarking data to allow performance predictions to be made.
    1.4. 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:
   4.1. 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.
   4.2. Release version 1.5.0, which will be under the new license chosen in 6.1. This release will include:
      - Fixes for two bugs that lead to bad crashes.
      - Introduce friendly naming format for jobs/recovery files.
      - Introduce automated cleanup of old recovery files.
      - Introduce better importing for developers.
      - Remove capitalisation of Longbow throughout codebase (source of major annoyance to developers)
      - New documentation for developers, i.e. an integration guide
   4.3. Support other project developers with Longbow integrations, such as integration with FESetup, ChemShell, Melody.
   4.4. 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.

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

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 – 2016 / 17 Plans (1 April 2016 – 31 March 2017)

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.

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

The Parallel Locator Exchange library (PLE) is provided as part of Code_Saturne. PLE can be used to couple any mesh-based codes (e.g. finite element, finite volume) and although coming from Code_Saturne this could equally be applicable to OpenFOAM and other CFD codes. PLE helps with the setup of MPI communicators and communication structures in order to extend current codes to include multi-scale and multi-physics capabilities, for example fluid-structure interaction or fluid and conjugate heat transfer, assuming that the meshes are in the same reference frame. It does not do the interpolation of values, for which the user has to provide a routine.

We will investigate and optimize the performance and scaling of the setup and communication of coupling with PLE, particularly the architecture of the library and the algorithms used.

Impact: this work will be of benefit to existing multi-scale and multi-physics users of the open source package Code_Saturne in the UK, for example on ARCHER, where Code_Saturne is installed as a module and is widely used. In addition the open source PLE library could be used in other codes as well.

Scalable High-Performance I/O

The increasing difference between the available I/O bandwidth and the required rate to sustain HPC applications, especially when considering exascale systems, results in system vendors further extending the storage hierarchy by inclusion of in-system storage in the form of burst buffers. Current and emerging hardware is increasingly using flash memory and Non-Volatile RAM (NVRAM) to provide a storage layer intermediate in performance between RAM and spinning disks. From the application level this can be thought of either as a secondary, slow memory or as a fast disk.

We will investigate how scientific applications can benefit from burst buffers for operations like checkpoint/restart, co-analysis of data, out-of-core algorithms, and integration with parallel I/O middleware (e.g. ADIOS). We will extend the initial investigations, which were made using the IBM BGAS system available in the STFC Hartree Centre, to other systems with different architectures and from other vendors: IBM NextScale, IBM POWER8, Cray DataWarp and DDN Infinite Memory Engine.

Impact: I/O has long been the Cinderella of parallel optimization, yet with data sizes growing it is becoming increasingly important. There is a need for information about parallel I/O techniques and especially to assess the new burst buffer / flash memory technology. How effective is it and how can it best be used from real large-scale applications? This has the potential to influence the data handling aspects of high-performance program design across the CCPs.

Power Optimization and Reduced Precision of Applications

The requirements to achieve exascale systems include power optimization. Existing programmes include research into power optimization for data centres, HPC systems, and at the level of the job scheduler. Current developments, e.g. the PowerAPI specification powerapi.sandia.gov, show an increasing inclusion of the application level in the power optimization process. Profiling tools such as TAU and Allinea MAP are now able to report energy-related metrics at the level of lines of source code making it possible to track energy usage in detail through an application. Many applications run with 64-bit precision throughout without really understanding whether this is necessary and in the past this has not been a significant performance issue. Not only do current processors offer an enhanced performance using reduced precision, but because of the reduced memory traffic, there is the prospect of much reduced energy consumption through using reduced precision. In some cases the whole application may be run with reduced precision, and in others it may be possible to limit the use of high precision to critical parts of the algorithm.

We will use profiling tools to investigate in detail the energy usage of a range of scientific applications. We will evaluate possible benefits of frequency scaling for memory bound or I/O intensive parts of the applications. We shall investigate a sample of algorithms and applications in order to determine whether these codes can operate at reduced precision, either in whole or in part. Having successfully investigated the energy usage and performance for the Jacobi Test Code using both single- and double-precision, we will look at a range of applications from different science areas employing different algorithms in order to investigate the energy characteristics of different algorithms and algorithmic variants. We shall use profiling tools to investigate the performance differences between full and reduced precision versions, both in terms of execution time and also in terms of energy usage.

Impact: the power consumed by HPC applications is becoming a matter of some concern and one which needs to be addressed across the CCPs. By using the latest techniques from energy efficient computing we will provide information back to the CCPs on how energy efficient their codes are and whether there are any immediate prospects for improving the energy efficiency. The technique of reducing precision without adversely affecting the quality of simulations is of great interest across the CCPs with the potential to reduce time to solution, energy usage, data transfer costs and data storage requirements.

Dissemination of Software Outlook results

The Software Outlook webpages will be regularly updated with information and results obtained through our work and also with links to useful information and news on our themes.

We will continue to issue bulletins periodically through the Software Outlook email bulletin.

We will issue shorter news items on Software Outlook research results and issues using the SCD Departmental Twitter feed.

We will setup a working group to report our findings to; the group will also provide guidance on the direction of future work plans. This group will consist of members of the CCP community who have an interest in the selected work packages. We already have expressions of interest from DL_POLY, DL_MESO and EPOCH developers in reduced precision. We are starting a conversation with CCP-WSI regarding code coupling and are planning a meeting in the coming month.

Project	Milestone	Target Date
Form Working Group	Identify candidates and invite to the group. We will hold an introduction meeting with each of the members to discuss the work plan they are interested in. *Task complete: working group formed and has met*	Q2 2016

	twice. Jeremy Yates has volunteered to test the Software Outlook audit. The working group like the idea of the webinars for training and Alin Elin is keen to do something on the co-array work.	
Code Coupling	Report on performance, scaling and optimization of code coupling using the PLE library included in Code_Saturne using an existing test case - coupling Code_Saturne either with itself or with a conjugate heat transfer simulation *Task complete: technical work packets are going well. MUI was identified as a potential alternative to PLE as it is better documented but eventually decided to look at a coupled problem from CCP-WSI..*	Q3 2016
Parallel I/O and burst buffers	Report on parallel I/O performance and capabilities using flash memory across a range of architectures *Task complete: this task was discussed at the last SLA steering committee meeting and the suggestion was to change to a training programme. Currently investigating the idea of creating webinars for training, which the working group liked.*	Q3 2016
Power Optimization and Reduced Precision	Report on power optimization of application codes *Task complete: Sue Thorne has been invited to speak at 2nd Workshop on Power Aware Computing in Germany where she will demonstrate the benefits of running mixed precision.*	Q4 2016
Power Optimization and Reduced Precision	Report on the performance and energy usage of algorithms and applications using full and reduced precision *Task complete: The technical report prepared by Sue Thorne was released in October Two DL_POLY reports are currently being prepared..*	Q1 2017
Working Group Meeting	Report on current results and seek feedback *Task complete: minutes circulated.*	Q3 2016
Software Outlook dissemination	Updating Software Outlook information on the SCD web pages; issuing email bulletins; tweeting on the SCD Twitter feed. *Task in progress: the Software Outlook web page needs updating and there is interest in moving over to a Drupal site to fit in with the other CCPs and HECs. Damian has requested a Drupal site so that Luke and Sue can start developing.*	Throughout the year

Staffing	**Effort**
Luke Mason	0.40 FTE
Sue Thorne	0.60 FTE
Andrew Taylor	1.00 FTE
Total	**2.00 FTE**

Software Outlook – Summary Report (1 April 2016 – 31 March 2017)

During this reporting year, Software Outlook mainly focussed on four projects: code coupling; power optimization and reduced precision; the setting-up of a Working Group to help direct future work

packages; investigating the possibility of developing a training programme. Following discussions with the SLA Steering committee, the work packet on parallel I/O was changed to the latter project and, in particular, we have been looking into the development of a series of webinars, which we hope to roll out during 2017-18.

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. Software Outlook's Coupling Project started in June with initial benchmarks run using CIAN2, a mini-app. This produced perfect weak and strong scaling as the problem size and number of processors increased: an accompanying technical report has been prepared. However, for real scientific codes, this perfect scaling is hard to reach. EDF's Code_Saturne contains a coupler, PLE, for use within Code_Saturne and external applications. Unfortunately, the documentation is extremely poor and, without significant, it would be very difficult for any of the CCPs to use it.

CCP-WSI are hare 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 are investigating the cause of this. CCP_WSI is a relatively new CCP and they have a number of different coupling scenarios. Through Software Outlook's involvement, we aim to make sure that these coupling aspects do not become a bottleneck in their simulations and, thus, reduce the execution times for their simulations. Given their simulations currently take many hours to compute, this will have a very positive impact on their work.

Power Optimization and Reduced Precision of Applications: The first work package for the year involved the completion of our investigations into whether the use of single precision instead of double precision can save time and energy when using a Blue Gene/Q system. The resounding answer was "yes, but only if there is a lot of data movement", see RAL Technical Report RAL-TR-2016-005 (http://purl.org/net/epubs/work/24764929). Working with the Hartree Centre's Energy Efficient Computing Group, we also carried out similar investigations on ARMv8 and Intel Xeon (IvyBridge) architectures: the results of this work will be reported at Power Aware Computing 2017, a workshop being held in Germany. The accompanying paper and slides will become publicly available afterwards.

During this year, our main focus has been the use of mixed precision within scientific applications. We started with an investigation into the energy consumption and execution times of HSL-MA79, a mixed precision software package for solving linear systems of equations (see Technical Report RAL-TR-2016-014 https://purl.org/net/epubs/work/30019264). The results gave us confidence that a mixed precision approach could be advantageous to the codes for a number of the CCPs with DL_POLY (CCP5) being offered as a candidate code. We have shown that mixed-precision can be used within the Fast Fourier Transform (FFT) component with little or no loss in the overall accuracy of the overall output. The total time spent performing the FFT component of the code decreases by up to 50%, giving an overall saving of 10% in the runtime of DL_POLY for some of the larger test problems. The use of mixed precision within other components has had mixed success. This work is in the process of being written-up and will also form the basis for some of our webinars.

Working Group: During the past year, one of our goals has been to make sure that the work we do is in line with the wishes of the CCPs. Working with the EPSRC, we set up a Working Group consisting of representatives from five different CCPs, with four of the representatives being external to STFC. The Working Group makes sure that our work packages are relevant and desirable with respect to the needs of the CCPs. The first meeting of the Working Group was held on 9th November and the

second meeting on 21st March. It will direct future work packages as well advise on how best to interact with the CCP community. Meetings are planned for every 6 months.

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

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

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.

Staffing	**Effort**
Luke Mason	0.40 FTE
Sue Thorne	0.60 FTE
Andrew Taylor	~~1.0~~ 0.79 FTE
Total	~~**2.0**~~ **1.79 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 cycle

At the renewal of the SLA in 2016, the yearly levels of resource agreed in principle over the period 2016/17 to 2020/21 were as follows:

Year	**16/7**	**17/8**	**18/9**	**19/20**	**20/1**
FTE	24.85	24.78	22.78	22.1	22.1

The total number of FTEs over the 5 year cycle is therefore 116.61.

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.

We therefore conclude that is the funding over this cycle will continue to follow the table above, there will be a relatively small amount of additional effort over this cycle, amounting to 3.61 FTEs. We have agreed with EPSRC that any plans to spend this extra resource will not be made at least until the 2018 international mid-term review. We have therefore not included this extra resource in our resource planning.

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

Please note that the above figures have been corrected to reflect that the total underspend for UKCP was 0.42 FTEs in 2016/17(instead of 0.5) because the 6 months of effort to compensate for Dominik Jochym's 6 month sickness leave, started in March 2016.

Planned Resource Profiles

Historically, resource planning was done over one year periods, based on the funding available for each project over a one-year window. Following discussions at previous meetings, starting from the year this report refers to, we are using a planning process which addresses the whole 5 years of the cycle. The longer planning period allows us to schedule staff deployment more effectively, and plan for recruitments more easily. In this new 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 cycle.

The following table shows the predicted spend profiling for the next five years with changes from the profile submitted in January 2017 highlighted yellow. For 2016/17 two figures are included – the planned effort originally submitted at the start of 2016/17 (in brackets) and the actual effort provided, which is marked in **red**.

	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)	2.25	~~2.25~~ 2.27	2.25	2.25	**11.25**
CCP5	0.42	3.20	1.95 (2.82)	~~3.56~~ 3.40	~~3.56~~ 4.00	~~3.56~~ 3.87	~~3.56~~ 3.20	**16.42**
CCP9	0.83	2.40	2.64 (2.71)	~~2.70~~ 2.20	~~2.81~~ 3.03	~~2.50~~ 2.56	~~2.24~~ 2.40	**12.83**
CCPmag	0.47	0.74	0.64 (0.83)	0.40	~~0.82~~ 1.10	~~1.40~~ 1.29	~~0.92~~ 0.74	**4.17**
CCPNC	1.80	1.30	1.62 (1.50)	2.00	2.00	~~1.80~~ 1.38	~~1.0~~ 1.3	**8.30**
CCPQ	0.00	1.86	1.69 (1.86)	~~1.86~~ 1.95	~~1.86~~ 1.90	~~1.86~~ 1.90	1.86	**9.30**
CCP Plasma	0.48	0.75	0.79 (1.00)	0.80	0.80	~~0.75~~ 0.80	~~0.60~~ 1.04	**4.23**
CCPi	0.33	1.20	0.82 (1.45)	1.50	1.43	~~1.30~~ 1.38	1.20	**6.33**

CCPPetMR	0.33	1.20	1.09 (1.15)	1.50	1.20	~~1.20~~ 1.34	~~1.25~~ 1.20	**6.33**
CCPBioSim	0.00	1.20	1.19 (1.16)	1.20	1.20	~~1.20~~ 1.21	1.20	**6.00**
MCC	0.00	2.50	2.53 (2.50)	~~2.50~~ 2.47	2.50	2.50	2.50	**12.50**
UKCP	0.42	1.00	1.36 (1.42)	1.00	1.00	~~1.00~~ 1.06	1.00	**5.42**
UK-COMES	0.00	1.00	0.93 (1.00)	1.00	1.00	~~1.00~~ 1.07	1.00	**5.00**
HEC Plasma	0.00	0.20	0.20 (0.20)	0.20	0.20	0.20	0.20	**1.00**
HECBioSim	0.50	1.00	0.98 (1.00)	1.00	~~1.10~~ 1.12	1.20	1.20	**5.50**
Software Outlook	0.10	2.00	2.31 (2.00)	~~2.00~~ 1.79	0.00	0.00	0.00	**4.10**
FTE TOTALS	~~**5.76**~~ **5.68**	**23.80**	**22.97 (24.86)**	~~**25.47**~~ **24.66**	~~**23.73**~~ **24.75**	~~**23.62**~~ **24.01**	~~**21.98**~~ **22.29**	**118.68**

2016/17 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 delivered are calculated and used to reprofile the effort and costing for future years.

The STFC project office calculated the yearly cost of the programme for 2016/17, based on the planned deployment of 24.85 FTEs, and taking into account current staff salary bands.

In total, 22.97 FTEs were delivered in 2016/17. The difference between delivered and planned resource for each project has been calculated and redistributed over future years so that by the end of the SLA cycle each projects will spend the amount of FTEs awarded for this cycle plus any historical underspend that project may have incurred.

2017/18 Planned Resource and Costing

[redacted]

The 2017/18 level of resourcing was planned to be 25.47 FTE in January (see 2017/18 Technical Appendix submitted in January). The up to date re-profiling shows a decrease in the planned level of resource for 2017/18, and a corresponding increase in later years.

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.

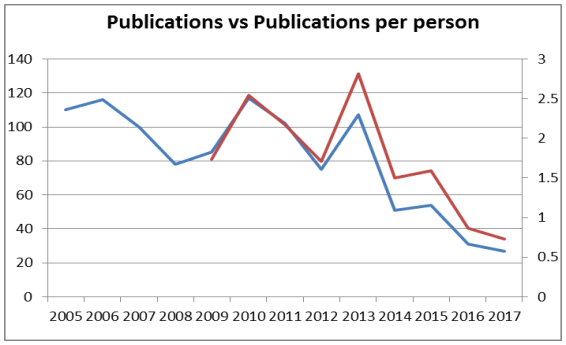
In the metrics graphs below, the blue line refers to the total number while the red line refers to the number per scientific/technical staff member. This is useful because metrics are included for any person irrespective of whether they are partially or fully funded by the SLA. For information, a graph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

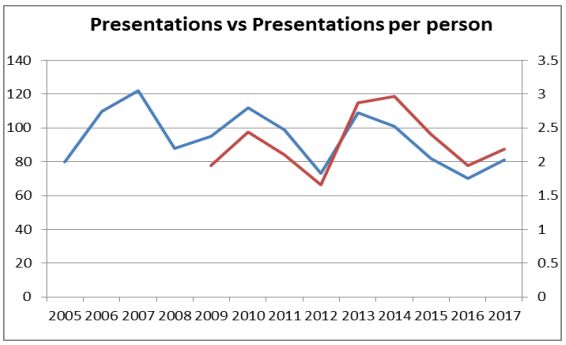
The citations metric shows an impressive upward trend, roughly doubling in the last four years to reach an average of roughly 60 citations per staff member. This is clear evidence of the success of the software supported by the programme. The considerable increase in the training days in recent years, 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. As a result, our staff have had to reduce the time spent on their own publications. This is part of the reason for the decrease in the publications metric in recent years.

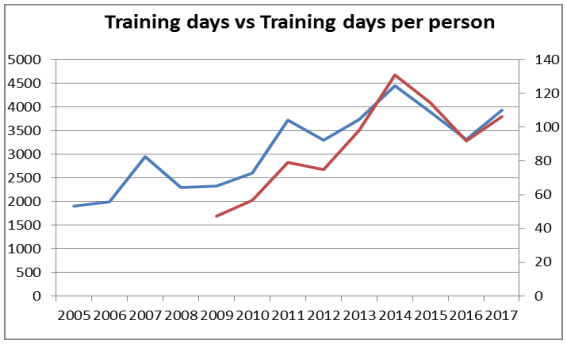
The reduction in the rate of publication has been discussed before. In many cases an initial publication will follow the development of a new computational procedure or algorithm in a supported code. In subsequent years the method or algorithm should be cited, but not published again; hence

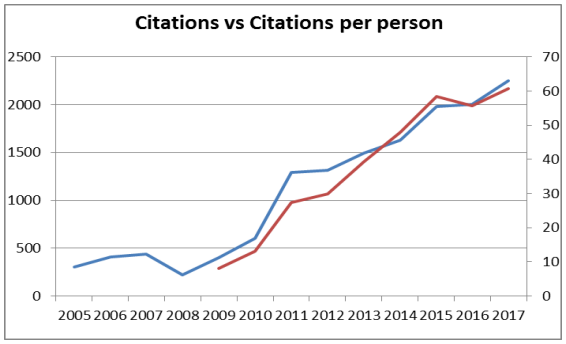
this trend shows the maturity of the code growth over time. Another factor that has contributed to the reduction in recent years is the loss of the long established and scientifically highly productive CCP12 project from our portfolio. In 2015, a number of new projects started which are staffed with relatively early-career staff and therefore will require some time to bed in enough to produce publications. Finally, the support requested by our communities in a number of relatively young projects involves mainly technical development and not publishable science. In future, we would expect community publications to include SLA funded staff as authors and we thank the Steering Committee and the CCP Steering Panel for the support given to the idea that the software developers behind community software deserve recognition.

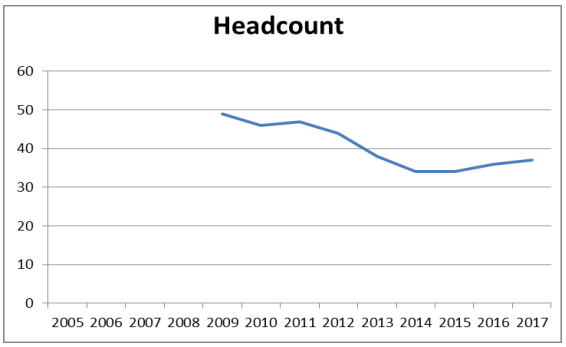
The presentations metric per person shows fluctuations around a roughly constant value. The headcount shows a significant drop from the mid 40s until 2012/13 to the mid 30s in more recent years.











Metrics breakdown by area

	FTE	Publications	Presentations	Training Days	Citations
CCP5 (including DL_ codes)	3.20	4.50	19.31	1003.80	709.00
CCP9	2.40	2.00	5.50	198.00	35.00
CCPmag	0.74	0.00	0.50	60.00	0.00
CCP-NC	1.30	1.00	1.00	175.00	1.00
CCPQ	1.86	3.00	3.00	52.50	84.00
CCP Plasma/HEC Plasma	0.95	4.00	1.00	32.00	95.00
CCPi	1.20	4.00	15.00	63.24	0.00
CCPPetMR	1.20	1.00	2.00	72.50	0.00
CCP-BioSim/HEC BioSim	2.20	1.00	6.00	88.00	7.00
MCC (including ChemShell, CRYSTAL)	2.50	3.50	21.16	1481.60	279.00
UKCP (including CASTEP)	1.00	0.00	3.00	500.00	1039.00
UK-COMES	1.00	2.00	3.49	210.20	0.00
Software Outlook	2.00	1.00	0.00	0.00	0.00
Totals		**27.00**	**80.96**	**3936.84**	**2249.00**

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

Appendix 1: Detailed 2017 / 18 Plans

Note: Changes to the draft plans submitted in January 2017 are highlighted yellow.

Project Office	Milestone	Target Date
	Attend CCP and HEC committee meetings as required	Ongoing
	Support CCP/HEC conferences and workshops as required	Ongoing
	Planning for the SLA International Review 2018	Ongoing
	Planning for TSM Backup software update	Ongoing
	Management of user access to data infrastructure	Ongoing
	Maintenance and monitoring of data infrastructure	Ongoing
	Management of SCD subnet in cooperation with CICT	Ongoing
	Provision of operation support (shifts) to Archer service	Ongoing
	Arrange internal project meetings with funded CCPs and HECs	Q2 2017
	Prepare and submit annual SLA report	Q2 2017
	Arrange and attend the CCP Steering Panel June meeting	Q2 2017
	Attend the SLA Steering Committee July meeting	Q2 2017
	Compile departmental data infrastructure usage data	Q2 2017
	Negotiate maintenance contract for data infrastructure hardware and software	Q2 2017
	Arrange internal project meetings with funded CCPs and HECs	Q3 2017
	Compile and submit ARCHER requirements	Q3 2017
	Create new CoSeC web site	Q3 2017
	Update TSM backup software for data infrastructure (prerequisite)	Q3 2017
	Prepare and submit mid-term SLA report	Q4 2017
	Create new CCP web site using Drupal	Q4 2017
	Arrange and attend the CCP Steering Panel December meeting	Q4 2017
	Attend the SLA Steering Committee December meeting	Q4 2017
	Update TSM backup software for data infrastructure (final version)	Q4 2017
	Procure new server for data infrastructure	Q4 2017
	Integrate new server for data infrastructure	Q1 2018
	Arrange internal project meetings with funded CCPs and HECs	Q1 2018
	Deliver presence at the Research Software Engineering Conference (Manchester)	Q3 2017
	Prepare 4 impact case studies	Q1 2018

CCP5	Milestone	Target Date
	Summer School organization & delivery.	Q2/Q3 2017
	Preparation of DL_MONTE workshop tutorials.	Q1 2017 and Q4 2017
	Release of new versions of software	Q1 2017 and Q4 2017
	Implementation of PPPM electrostatics	Q4 2017
	Advanced mesoscale course at Summer School	Q3 2017
	DL_FIELD to create DL_MONTE files.	Q3 2017
	Expansion of DL_F notation to amino acids	Q3 2017
	Multiple potential capability	Q1 2018
	Improve features for inorganic systems (e.g. freeze)	Q4 2017
	Improvement of bio-inorganic system models (e.g. auto mixing of	Q4 2017

	VdW parameters)	
	New release of DL_POLY	Q1/Q2 2017
	Preliminary investigation of Gay-Berne potentials + strategy plan for implementation	Q2/Q3 2017
	Prototype of Gay-Berne programs	Q4 2017
	Training event for ChemShell for CCP5	Q4 2017
	Preliminary investigation of empirical valence bond + strategy plan for implementation	Q3/Q4 2017
	Develop web presence as more interactive – web forms/distro etc	Ongoing
	DL_Software @QMUL	Q1 2017
	Hold a DL_Software training event at the University of Strathclyde	Q4 2017
	Identify a venue and date for the "Experimentalist & Industrialists" workshop to be held late 2018	Q4 2017

CCP9	**Milestone**	**Target Date**
	Submit Rare earth doped ceria article	Q1 2018
	Workshop: LMF-QSGW hands-on course	Q2 2017
	Workshop: KKR hands-on course	Q1 2018
	Flexible atomic solver in FPLMTO, technical report	Q3 2017
	Collaboration with Julie Staunton on permanent magnet materials, visit and discussion	ongoing
	Results magnetic properties of GdCo5	Q4 2017
	V&V for the elements (if successful project will extend to lanthanides, Q3 2017)	Q2 2017
	Submit results on Ab initio magnetism of Mn3Sn (collaboration)	Q3 2017
	Publish article on magnetism in Gd-alloys	Q4 2017
	Deliver capability to evaluate CF parameters in LMF (collaboration)	Q2 2017
	Results on TM-oxides	~~Q3 2017~~ Q4 2017
	Workshop on atomistic simulations of nuclear materials	~~Q4 2017~~ Q1 2018
	Organize CCP9 working group meeting	Q2 2017
	Implementation of SIC in LMF; initial phase	Q2 2017
	Implementation of SIC in LMF; demonstration	Q1 2018
	~~Local SIC implementation in KKR~~	~~Q1 2018~~

CCP-mag	NMAG installation procedure	Q2 2017
	Co-ordinate session at IOP Magnetism 2017	Q2 2017
	Finalize data structure for geometry	Q3 2017
	Finalize data structure for exchange couplings and anisotropies	Q3 2017
	Implementation of basic infrastructure of ESCDF library	Q4 2017
	Run KKR course (joint with CCP9)	Q1 2018
	Continued support for ISIS	ongoing

CCP-NC	**Milestone**	**Target Date**
	Moving Soprano from alpha to beta stage (SS)	Q4 2017
	Inclusion in CASTEP of the Tran-Blaha functional (AB)	Q4 2017

	Release with CASTEP of the NICS tool (SS)	Q4 2017
	Development of a prototype of an NMR database (AB)	Q2 2017
	Integration of MagresView with said database (SS)	Q2 2017
	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)	~~Q3 2017~~ Q1 2018
	Testing and assessment of the feasibility of machine-learning techniques with regards to NMR parameter prediction, esp. in organic molecular crystals (AB)	Q1 2018
	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)	Q3 2017
	Upgrade and maintenance of the CCP-NC website and its content (SS, AB)	ongoing
	MagresView code maintenance and extension (SS)	ongoing

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. 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).	Q2-Q3 2017
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.	Q2 2017
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).	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.	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).	Q2 2017

TNT	DJ to set up webpage for online payment for 'Windsor 2017' cold atoms /strongly-correlated-systems workshop.	Q2 2017
TNT	To be lead by SEG following SL's return from sick leave, consultation with Oxford/Bath (and UCL) to review TNT (and CCE) support needs (SEG, MP AGS). If appropriate: upgraded TNT Python interface work (SL). Plans for joining SESC Build Service (SL).	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).	Q2 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.	Q2 2017- Q4 2017 (publications list set-up), general support continuous
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).	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).	Q3 2017
UKRMol+	DJ to support (via web bookings) the planned Quantemol UKRMol+ training day as required	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).	Q3 2017 - Q4 2017
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. SL to provide SESC support for QUB codes as requested.	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.	Q3 2017 (into Q4 2017)
TNT	SEG (SL) to commence active support for TNT/CCE as decided in earlier review meeting.	Q3 2017- Q4 2017
SBS support	SL to work (separately) with TNT and UKRMol+ (in conjunction with Flagship or as core support) on Build Service integration.	Q3 2017- Q1 2018
Novel Technology/ PFARM	Continued novel technology software support as deemed relevant/important (details to be added/reported).	Q3 2017 (into Q1 2018)
Antimatter	Continued advice/support for MML and student (MP) as decided in Q2 meeting (details to be added)	Q3 2017 (into Q4 2017)

General	General website and other support, as above. Review of objectives.	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)	Q4 2017 – Q1 2017
QUANTICS and TNT	Continued support for Quantics and TNT as decided in Q3 review (SL).	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
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 (se above). Details to be added.	Q4 2017 – Q1 2018
General	Implementation of agreed longer term objectives from Q2-Q3 2017	Q4 2017-Q1 2018

CCPPlasma	**Milestone**	**Target Date**
	~~GS2: Design and implement a test code to assess the speed and scaling of routines for memory redistributions between the various memory layouts.~~ 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.	Q2 2017
	~~BOUT++: Assess the performance of the OpenMP parallelization on Archer.~~ BOUT++: Optimize the DataIterator object in BOUT++. Parallelize with OpenMP and ensure that it is vectorized by compilers.	Q3 2017
	~~GS2: Optimize/reimplement memory redistribution routines in light of findings from test code.~~ 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.	Q4 2017
	~~BOUT++: Improve existing Python tools and provide a Python wrapper for the BOUT library.~~ 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.	Q1 2018

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.	Ongoing

	Assist in new proposal writing.	
	Embed framework: ISIS/IMAT– working with ULTRA and Phase 2 opens access up to users	Q4 2017
	Embed framework: DLS/savu – Working on SCARF integration and Phase 2 considers new beamline users	Q3 2017
	Embed lab based framework: UoM/ UoS/ UoW	Ongoing – case studies due Q3 2017
	Add quantitative code examples from the community: see mid-term targets.	Q4 2017
	Add pre-processing stages beamhardening correction experiments; now to include publications.	Q1 2018
	Organise the main ToScA conference; September 2017	Q3 2017
	Set up and run continuous build and test system in CCPForge	Ongoing
	Optional: Iterative code for the Nikon XTek X-Ray CT accelerated versions (Link/use tier 1 or tier 2 HPC)	Q3 2017
	Optional: Optimise projection algorithms from community requests	Q1 2018

CCPPET-MR	Milestone	Target Date
	~~Website, mailing lists, source code and data archives~~ 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 event sessions	Ongoing
	Support current training courses and organise developer workshops	Ongoing
	Assist in new proposal writing.	Ongoing
	~~Populate database for both simulated and acquired data (i.e. framework, will slowly be filled over the project). Links to be made with DPUK site.~~	~~Ongoing~~
	~~Visit sites in the network to gain experience with a few selected packages for image reconstruction. Embedding within the main groups STiR and Gadgetron~~ Visit sites in the network to gain experience with a few selected packages for image reconstruction and to get others started with SIRF	Ongoing – embedding two days a week
	Set up and run continuous build and test system in CCPForge	Ongoing
	~~STiR code – API release (MATLAB or python) User release~~	~~Q3 2017~~
	~~Gadgetron code – API release (MATLAB or python) User release~~	~~Q3 2017~~
	~~STiR and Gadgetron combined User release~~	~~Q1 2018~~
	SIRF Release 0.9.	12 May 2017
	Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide.	Ongoing
	More real data functionality (import of raw data, PET randoms, norm and scatter), excluding GE raw MR data.	Ongoing
	~~Optional: Profiling and (if necessary speed-up) of 1 PET and 1 MR image reconstruction package~~ Optional: Profiling (and possibly speed-up) of PET reconstruction.	Ongoing
	~~Optional: Creation and maintenance of test-cases of PET/MR data and reconstructions – link to releases~~	~~Q1 2018~~

	Write SIRF installation script for Windows, possibly using pre-compiled libraries.	Q3 2017
	SIRF Release 1.0.	Q4 2017
	Implement image data transformations between PET and MR and between different voxel grids and encapsulate image data into common SIRF image object.	Q1 2018
	Implement PET reconstruction with MR anatomical priors.	Q1 2018
	Implement iterative MR reconstruction with Gadgetron.	Q2 2018
	SIRF Release 2.0	Q2 2018

CCPBioSim	Milestone	Target Date
TWK	Hold ChemShell training workshop for biomolecular QM/MM modelling	Q2 2017
TWK	Lead organisation of the 3rd CCPBioSim/CCP5 Multiscale Modelling Conference	Ongoing (to be held Q2 2018)
HHL	LOMAP2 integration	Q3 2017
HHL	Longbow integration	Q2 2017
HHL	ProtoMS support	Q2 2017
HHL	Support for side chain mutations (FESetup 2.0)	Q1 2018
HHL	General clean-up and usability improvements	Q4 2017

MCC	Milestone	Target Date
ChemShell / DL_FIND	(Supervision of ChemShell work package in MCC flagship project – subject to funding decision)	Ongoing
	Implementation of freeze and thaw frozen density fragment optimisation in Python-ChemShell	Q1 2018
	Improve usability of nudged elastic band method in DL-FIND through improved initial path guesses, optimisation diagnostics and additional tutorials	Q3 2017
	Support for ChemShell and GAMESS-UK 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	Onoging
	Collaboration with Graeme Day on real examples of organic crystals MD modelling using multipolar FFs and self-polarisable multipolar FFs.	Q2 2017
	Preparation and lectures of DL_POLY_4 at DL_Software workshops	Ongoing
	Support for DL_POLY_4 on ARCHER (ITT). Support for DL_FIELD (CY)	Ongoing
CRYSTAL	Merge of UK and Italy version of CRYSTAL17 for release	Q2 2017
	Paper on multiferroic GaFeO3 – in collaboration with N. Harrison and R. Cernik	Q2 2017
	Paper on dynamics of molecules in solution – in collaboration with T. Parker and R. Bisby	Q2 2017
	Compilation and testing of CRYSTAL17 on Archer and STFC clusters	Q2 2017
	Tests of massively parallel version of CRYSTAL17 on large disordered systems. In collaboration with Dr I Bush (Oxford	Q2 2017

	University)	
	LB to visit Turin University for discussion about current CRYSTAL developments.	Q2 2017
	Draft of paper on dynamics of catalytic molecules in solution, in collaboration with ISIS. (Dr N Holzmann and LB)	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.	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)	Q2 2017
	LB to deliver 4 lectures and 3 half-day tutorials at CCP5 summer school on molecular simulation at Lancaster University.	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)	Q3 2017
	Organise MSSC2017 CRYSTAL summer school and Imperial College London and deliver 5-6 lectures (TBC) and tutorials.	Q3 2017
	Work on massively version of CRYSTAL17 to be extended (potentially) to biological samples. Compile list of potential systems to be considered and set up calculations.	Q1 2018

UKCP	**Milestone**	**Target Date**
	Consolidation of CASTEP's Raman and NLO "2n+1" code: including symmetry, calculation checkpoints, optimisation, and post-processing tools	Q2 2017
	Produce specification for post-processing tools based on the CASTEP Python interface	Q2 2017
	Bring SESC's Jenkins CI system into production for CASTEP, superseding buildbot	Q3 2017
	Co-organization and teaching of CASTEP workshop in Oxford	Q3 2017
	Organisation of 2018 CASTEP "codefest" core developer workshop	Q4 2017
	Trial and produce an electronic license management system for academic CASTEP	Q4 2017
	Release management of CASTEP 18 including documentation and liaison with major HPC services	Q4 2017
	~~Investigate extension of CASTEP's "2n+1" code for structure optimisation based on observable quantities~~	~~Q1 2018~~
	Code CASTEP on-the-fly pseudopotentials for exact exchange based on Stewart Clark's "Local Fock Exchange"	Q1 2018

UK-COMES	**Milestone**	**Target Date**
JM	Prepare documentation of the OPS-based code for application developers	Q2 2017
MS/JM	Implementation of immersed boundary method	Q3 2017
JM/MS	Continue developing the OPS-based code; release a workable 2D version and start testing the 3D case.	Q4 2017

MS	Implementation of contact angle hysteresis	Q1 2018

HECBioSim	Milestone	Target Date
	Webpage modifications	Q2 2017
	Benchmarking study with webapplet for data	~~Q2 2017~~ Q3 2017
	Deliver Longbow version 1.5.0 (4.2 above)	Q3 2017
	Chemshell – Longbow integration	~~Q3 2017~~ Q4 2017
	3 research highlights	~~Q4 2017~~ Q1 2018

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.	Q2 2017
	Work packet revolving around FLAME from CCP-Plasma	Q3 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.	Q4 2017
	Investigating the effects of using mixed-precision approaches on novel architectures available within the Hartree Centre	Q1 2018
	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	Q2 2017
	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 during the simulation is terrible. How can it be improved? Test examples to be provided by CCP-WSI	Q1 2018
	Software Audit of CCP Software	Q1 2018

Appendix 2: Highlight Papers

CCP5

C. W. Yong, 'Descriptions and implementations of DL_F Notation: A natural chemical expression system of atom types for molecular simulations' Journal of Chem. Info. Modell. doi:10.1021/acs.jcim.6b00323

J.A. Purton, N.L. Allan and D.S.D. Gunn, 'Simulation of doped CeO2 at finite concentrations', Solid State Ionics, 299, 32-37 (2017).

CCP9

Rare-earth pnictides and chalcogenides from first-principles, J. Phys.: Condens. Matter 28 (2016) 223001.

CCP-NC

Simone Sturniolo, Timothy F.G. Green, Robert M. Hanson, Miri Zilka, Keith Refsona, Paul Hodgkinson, Steven P. Brown, Jonathan R. Yates, Visualization and processing of computed solid-state NMR parameters: MagresView and MagresPython, SSNMR 78 (2016) pp 64-70

CCPQ

EAG Armour and M Plummer, Calculation of the resonant contribution to Zeff(k0) using close-coupled equations for positron-molecule scattering, J. Phys. B At. Mol. Opt. Phy. 49(15), 154003, 2016 (doi:10.1088/0953-4075/49/15/154003)

CCPPlasma / HECPlasma

L. Anton, C. M. Roach, L. F. van Wyk, E. G. Highcock and J. T. Parker, Enhancing scalability of the gyrokinetic code GS2 by using MPI Shared Memory for FFTs, Proceedings of the Cray User Group Conference (2016)
https://cug.org/proceedings/cug2016_proceedings/includes/files/pap124.pdf

MCC

A.J. Logsdail, C.A. Downing, T.W. Keal, P. Sherwood, A.A. Sokol and C.R.A. Catlow, Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces, Phys. Chem. Chem. Phys., 18, 28648 (2016)

UK-COMES

M. Ashworth, J. Meng, V. Novakovic and S. Siso, Early Application Performance at the Hartree Centre with the OpenPOWER Architecture, pp. 173–187 in Proceedings for High Performance Computing: ISC High Performance 2016 International Workshops, Frankfurt (2016)

Peng Y, Zhang JM, Meng JP. Second order force scheme for lattice Boltzmann model of shallow water flows, accepted by Journal of Hydraulic Research, and published online http://dx.doi.org/10.1080/00221686.2017.1286392

Appendix 3: Major Code Developments

Code	Highlight	Comments
CCP5		
DL_POLY	• Implementation of core-shell polarisation for beyond point charge atoms (multipolar electrostatics). The performance of the conditionally updated Verlet Neighbour List feature has also been improved to give a larger and longer range of conditional availability to the user. • Further developments include: CHARMM model enablement for self-induced polarisation of intra-molecular interactions, improved core-shell filtering, new "zero K fire" optimisation option that is independent on system target temperature, etc. • A release date was planned for Q1 2017 but is now moved to Q2/3 2017.	• Complete • Complete
DL_FIELD **DL_ANALYSER**	• Introduce CVFF, implements universal atom typing description (DL_F Notation) • Program restructuring to improve efficiency • Release of DL_FIELD 3.5 • Multiple-potential calling and mixing capability • Extension of DL_F Notation to other FFs other than PDB • Multiscale work flow activities. • Implementation of the DL_F atom type notation, efficiency improvements and potential mixing capabilities. Work has gone into introducing CVFF, a general consistent force field that implements universal DL_F atom typing description (DL_F Notation). • The program has been restructured to improve efficiency. Multiple-potential calling and mixing capability has been introduced which works for both organic/organic and organic/inorganic systems. It is currently only handling PDB input structures and work is ongoing to extend this. Extension of DL_F Notation to other FFs is also on the way. This includes major rearrangement of library files, for instance separation of CHARMM force fields into independent multiple components. The outreach multiscale work-flow activity, using SDS (sodium dodecyl sulphate) as a case study, is ongoing – it involves setting up the Gromacs' united atom FF model, G54A7.	• Complete • Complete • Complete • Complete • Complete • Complete • Complete • Complete
DL_MESO	• Smooth particle mesh Ewald • Widom insertion • OpenMP optimization • Release of version 2.7 • Created Widom insertion post-processing utility for excess chemical potential calculations (completed Q3 2016). Implementation of SPME in DL_MESO_DPD	• Complete • Complete • Complete • Postponed to Q1 2017 • Complete

	(completed Q4 2016). Release of DL_MESO version 2.7 was due in Q1 2017 but now moved for Q2/3 2017.	
DL_MONTE	• Free Energy/ Lattice Switch MC • MC for Metallic systems • Improved Manual • Q1 Release of new version • Extra functionalities added to DL_MONTE: Free Energy Difference (FED) methods, lattice and phase switch, extra volume moves (e.g. in log space), user-defined VdW forms, improved input/output (e.g. DCD format), revised Ewald summation and improved performance. The manual was also updated and improved.	• Complete • Complete • Complete • Completed in Q2 2016 • Complete
Chemshell	• Improvements in tutorials • Code revisions to support Tcl 8.6 • Improvements to the ChemShell tutorial following the 2016 workshops were carried out and a new release of Tcl-ChemShell (3.7) is targeted for 2017.	• Ongoing • Complete • Complete

CCP9

Lmf (LMTO)	Implementation of gradient corrections in potential (CCP9)	Complete
QSGW (based on lmf)	• HDF5 I/O implementation (eCSE). • Memory distribution via PBLAS/ScaLAPACK (eCSE) • Further optimization of routines (CCP9)	• Complete • Complete • Complete
CRYSTAL	• Implementation and testing of a full projector method (eCSE) • Merge of the current UK developer version with the master code (CCP9)	• Complete • Complete

CCP-NC

Soprano	• Full first public alpha release; • Integration with ASE and Scipy for loading and clustering of large amounts of chemical structures; • Integration with GULP for support of empirical force fields; • Integration with HPC systems through interfacing with common queueing systems (Grid Engine, LSF, PBS) and support for daemon Submitter processes	• Complete • Complete • Complete (experimental) • Complete (experimental)
CASTEP	Novel Tran-Blaha XC functional for improved NMR ab-initio calculations	Early stage development

CCPQ

TIMEDEL	Additional functionality added for calculating resonance branching ratios across a resonance in addition to peak values	Complete
TNT	The latest virtual machine implementation of TNT ported to CCPForge (too large for standard upload)	Complete

UKRmol/UKRmol+	• SEG port to continuous integration. • Re-indexing optimization of (continuum) atomic orbitals in 2-electron integrals • Re-indexing optimization of (continuum) molecular orbitals in 2-electron integrals	• Underway as scheduled • Complete • Underway as scheduled
RMT	SEG restructuring of code for CCPForge (and later CIT) port	Complete (restructuring and CCPForge port)
PRMAT	Additional flexibility added for special cases with some 'all-core' symmetries	Complete

CCPPlasma / HECPlasma

GS2	• Implementation of collision term module which uses the same memory layout as the field solve module. • New implementation of GS2 collisions model.	• Complete • Complete
BOUT++	• Implementation of IMEX solver in CCFE physics module. • Release of BOUT++ v 4.0.0 • Implementation of linearized version of CCFE's physics module STORM • Implementation of implicit-explicit solver in STORM.	• Complete • Complete • Complete • • Complete
EPOCH	The EPOCH project was awarded a software development project by EPSRC (EP/P02212X/1) for two years starting in September 2017. The appointed PDRA (Heather Ratcliffe) will join Warwick's new RSE group on a longer contract and be seconded to the EPOCH fulltime for the 24 of this award.	

CCPi

CCPi quant	• Mainly maintenance: Updated versions for new underlying software versions. • Amira data loader scripts added.	• Ongoing • Complete: instructions at http://www.ccpi.ac.uk/node/200
CCPi pre	VBA Coding for Nikon X-Ray CT Machines: This is developed by Parmesh Gajjar at Manchester University. Code is available at: https://ccpforge.cse.rl.ac.uk/gf/project/vba_nikonxrayct/	This is hacking code to customize Nikon X-Ray CT machines; to automate and customize the CT machines parameters such as X-Ray source, the manipulator and the image processing.
CCPi post	Tomography beam hardening codeCode is available at https://ccpforge.cse.rl.ac.uk/gf/project/tomo_bhc/	Beam hardening correction code is being developed by Dr Ronald Fowler based on work from Dr G R Davis ,Queen Mary University London.

CCPPetMR

CCPPETMR VM	Virtual Machine with pre-installed CCPPETMR software	Ongoing and also stored on dropbox and main website
iUtilities	Core interface building utilities	Core utility codes released prior to two main packages; xGadgetron and xSTIR. Debugging is ongoing.

xGadgetron	Gadgetron interfaces to C, Python and Matlab	Developers' release submitted in Q3 2016
xSTIR	STiR interfaces to C, Python and Matlab	Developers' release submitted in Q3 2016
SIRF	• Remove code overlap in C interfaces to STIR and Gadgetron by creating common interface utilities project. • Make demo scripts more user-friendly by using docopt package (in Python), inline help and next-user-action prompts. • Bring STIR and Gadgetron interfaces under one roof by creating SIRF project on GitHub. • Create a separate GitHub project for large data files and move to it SIRF raw data files. • Provide basic-user-friendly inline documentation in demo scripts and more detailed documentation in Python and Matlab interface modules. • Write Users Guide targeted at a basic user. • Provide cross-platform CMake-installation instructions. • Provide full installation script (to install SIRF, STIR, Gadgetron and dependencies).	• Complete • Complete • Complete • Complete • Complete • Complete • Complete for Linux, Windows installation requires user's effort • Complete for Linux and MacOS
All code is now centralised on: https://github.com/CCPPETMR/. Ismrmrd – ISMRMRD Raw Data Format and python tools as well as Siemens converter are also included on the CCP PETMR github repository.		

CCPBioSim

FESetup	• Release of FESetup v1.2, including improvements to support for CHARMM, Amber, Gromacs and Sire, and support for GAFF2 • Alchemical analysis tool: improvements to AMBER parser and prototype for NAMD support • LOMAP: new prototype code as basis for rewrite of the code • Prototype for analysis of work integrals in non-equilibrium alchemical free energy simulations • Support for ProtoMS in FESetup	• Complete • Complete • Prototype complete • Prototype complete • Code review underway

MCC

ChemShell	• Integration of GULP force field scripts • ChemShell I/O support in Aten • Parallel MPI framework in Python-ChemShell • LSDalton direct linking in Python-ChemShell	• Complete • Completed as planned (Q1 2017) • Complete • Ongoing (targeting Q1 2017)

UK-COMES

DL_MESO_LBE	• Cascaded Lattice Boltzmann collisions (including implementation of Guo-based forcing) • Outflow boundary conditions and further options for boundary conditions (Inamuro, Zou/He, regularised) • Solid/fluid interactions via Ladd algorithm (solid suspensions) • Testing the OPS library	• Completed • Outflow conditions complete, others in progress (due to be completed Q4 2016) • In progress, should be completed Q1 2017 • Tested successfully. The code

		has been continually developed, and a workable version will be released in next report period.
	• Large Eddy Simulation (LES) model for turbulent flow	• In progress, should be implemented into the OPS-based code in Q1 2017.
DL_MESO	• Cascaded lattice Boltzmann collisions	• Complete
	• Additional types of boundary condition specifying fluid velocities or densities for planar surfaces (Zou/He, Inamuro, regularised)	• Complete
	• Oscillating boundary velocities and forces	• Complete
	• Implementation of suspended solid particles in fluid using Ladd algorithm	• Ongoing (to be completed in Q2 2017)
OPS LBE Code	• Creation of two-dimensional LBE code to use OPS libraries	• Complete
	• Testing of code on various architectures	• Complete
	• Implementation of four wall boundary conditions (Zou-He, non-equilibrium extrapolation, kinetic, bounce-back)	• Complete
	• Implementation of extrapolated inflow and outflow boundary conditions	• Completed
	• Testing the above boundary conditions for pressure-driven flow and flow around a square	• To be finished soon (a paper is undergoing revision)
	• Preparation of documentation for application developers	• Ongoing (due for completion in Q2 2017)
	• Releasing the 2D code	• Ongoing (copyright issues currently under discussion)

HEC-BioSim

Longbow	• Recovery mode – to recover and reconnect with running jobs if Longbow crashes.	• Complete
	• Dis-connectable/Re-connectable sessions to eliminate the need to be persistently connected.	• Complete
	• Added ability to call scripts as part of final submission process.	• Complete
	• Implemented sub-queueing, Longbow will maintain its own queue in cases where the machine has a slot limit and submit them as slots open up. This limit is detected automatically.	• Complete
	• Added support for a limited number of accelerators and their special directives under some schedulers.	• Complete
	• Longbow has been refactored such that continous integration principles can be readily applied. Over 600 unit tests have been written which are now auto executed and their coverage measured each time a commit hits the git repository. This leads to higher quality code and a structured method to work with other developers	• Complete
GPCR GLAS	Basic GLAS algorithm developed in python still requires work on GPCR indexing algorithm.	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. In 2016-2017 this accumulated to work with 5 PhD students over 5 UK institutions over a month's worth of collaborative work visits with the most significant one by Galvin Khara (UCL) visiting STFC for one week to work on the Two Temperature Model advancements in DL_POLY_4.

- 'Introduction to Molecular Simulation' @ Altrincham Grammar School for Girls (Y13 students) – May 2016 (presented by CY).
- DL_FIELD talk and tutorials @UCL in April 2016 (CY).
- 2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems. Manchester, 13-15 April 2016 – 92 attendees (TK co-organised).
- DL_Software Training and Hack Day @ NSCCS Imperial College, 18-20 April 2016 – 20 participants for training and 7 for the Hack Day (organised by CY & ITT).
- CCP5 Summer School 2016 @ Lancaster University – 10-19 July 2016 (organised by JAP) organised and lectured. The chair had to pull out due to family reasons and JAP took over the lead at the practical sessions, MS co-lectured the mesoscale advanced course.
- CCP5 Annual Meeting and Industry Day 2016 @ Harper Adams University – 12-14 September 2016. The industry day was held in conjunction with the RSC (organised by JAP). 55 attendees. JAP presented 2 posters and CY 1 poster at this event.
- Simulations for the experimentalist and the industrialist (with input from CCP_BioSim) @ Diamond Light Source – 15-16 November 2016. This is a new initiative, it was fully subscribed with 25 attendees (organised by JAP, ITT and CCP5 Chair). IT, TK, CY, MS, JAP gave talks.
- MC and HMC talk @ the Energy Materials Consortium Meeting in Bath – September 2016 (JAP).
- "HPC software as infrastructure and tools for modelling soft condensed matter": invited presentation at N8 HPC workshop @ University of Manchester –12 April 2016 (MS substituting ITT "Unveiling the impact of HPC in soft condensed matter").
- "General Purpose Multipolar Electrostatics within Domain Decomposition" presentation by ITT (invited speaker) CECAM Workshop "Beyond point charges" @ CECAM, Lausanne – 4-7 April, 2016.
- "DL_POLY_4 Multipolar Electrostatics" presentation by ITT (invited speaker) at the Advanced Potential Energy Surfaces Symposium (PHYS division ACS-2016-PHILLY), USA – 21-25 August, 2016.
- Output to EPSRC Software Strategy Workshop @ London – October 2016 (ITT).
- "Evolution and revolution: optimising mesoscale modelling codes for Intel Xeon Phi": presentation at PRACE Technical Training School "Code Modernisation for Intel Multi Core and Xeon Phi Architectures" @ NCSC, Sofia – 25–28 April 2016 (MS).

- Molecular Simulation Methods and Capabilities at CCG, Daresbury Laboratory, presentation at the Faculty of Chemistry, University of Sofia – 25–28 April 2016 (ITT).
- A DL_Software & Hack Day events were undertaken, at STFC Daresbury Laboratory in December (25 participants).
- For the first time we ran a new course “Simulations for the Experimentalist and Industrialist”, organised by John Purton, Ilian Todorov and the CCP5 Chair. It was held at the Diamond Light Source (15-16 November 2016) and included additional input from representatives from CCPBioSim, HEC-MCC, and invited presentations from UCL, Diamond and ISIS. This new event was fully subscribed, with 25 attendees and well received by experimentalists from ISIS, Diamond and institutions abroad as well as industrialists from Syngenta. We plan to repeat this course in 2018.
- Community outreach and networking were facilitated by transitioning the old CCP5 website and release after considerable contents restructuring within a new Drupal Content Management System hosted on virtual Apache server based at RAL. This work was mainly carried out by Chin Yong.
- Computational Chemistry material from CCP5 and STFC Computational Chemistry group modelling research was gathered and listed by Ilian Todorov at ftp://ftp.dl.ac.uk/ccp5/DL_POLY/Outreach/ for outreach purposes to be developed further by Tim Harrison, Director of Outreach, Chemistry, Bristol.
- The CCP5 international visitor program continued with a tour by Mark Tuckerman (New York University) in March & April 2017 (hosted by Ilian Todorov).

CCP5 Sponsored events

- CCP5 Workshop on HPC in Soft Condensed Matter @ Manchester – 12 April 2016 (20 attendees).
- Computer Simulation of Radiation Effects in Solids (COSIRES) @ Loughborough – 19-24 June 2016.
- Energy Materials Consortium Symposium @ Bath in September 2016
- First International RSE Conference @ Manchester – September 2016 (210 attendees).
- Hermes Summer School 2016 @ Windsor Great Park – 27-31 July 2016.
- Methods to Simulate Nucleation and Growth from Solution (MSNGS) @ University of Sheffield – 4-5 August 2016.
- CCP5 summer bursaries 2016 awarded to students at Bath (supervisor Alison Walker), Sheffield (supervisor Colin Freeman), Bristol (supervisor Natalie Fey), Lancaster (supervisor Jamshed Anwar), Nottingham (supervisor Jonathan Hirst). We plan to update the rules for 2017 to include “teaching and outreach material” using CCP5 software.

CCP5 visitors (visited and invited)

- Mark Tuckerman and Martin Schoen have accepted invitations for 2017.

CCP9

- In September the biannual Psi-k/CCP9/CECAM graduate school was held at Daresbury Laboratory, with lectures on DFT, and the codes ABINIT, ELK, SIESTA and YAMBO. 18 students took part in the school.
- Mike Payne, Leon Petit & Jerome Jackson organized the "State of the Art in Electronic Structure" E-CAM workshop, which took place in September in Cranage Hall. A report on the workshop has been written and submitted to E-CAM.
- The joint CCP-mag/CCP9/EUSpec SPR-KKR Hands-on course was held at Daresbury Laboratory from 14 November until 17 November. It was well attended with 24 trainees. Martin Lueders gave three lectures on DFT and magnetism.

- Martin Lueders gave a series of lectures on electronic structure at the EPSRC/IOP summer school "Physics by the Lake", which was held in July at Cumberland Lodge.
- Martin Lueders presented the collaborative work on magnetocaloric materials at the JEMS2016 conference.
- The CCP9 Young researchers meeting 2016 was organized by Yvette Hancock in York, 18-19 July. There were 45 registered participants. Event highlights included keynote and recently appointed academic presentations detailing background theory and applications.
- Leon Petit presented the work on Gd-intermetallics talks at TEMM2016 (invited) in RAL 16-17 June, at the International Conference on Magnetic Materials and Applications (invited),1-3 February 2017, Hyderabad, India and at the AVS 63rd International Symposium and Exhibition, Nashville, 6-11 of November. Leon also gave a seminar on DLM-SIC at Oak Ridge National Laboratory on 15th of November.
- Jerome Jackson presented an overview of the SIC-LSD methodology at the ETSF workshop in Lund, 20-23 September 2016, and at the Simons Summer School on the Correlated Electron Problem, 20-22 May 2016, Cumberland Lodge.
- Barry Searle was instructor at Workshop on Electronic Structure Software for Periodic Systems in Daresbury in January 2016, and was instructor at MSSC2016 CRYSTAL school at Imperial College London in September 2016

CCP9 furthermore provided funding for:

- CASINO hands-on course “Quantum Monte Carlo and the CASINO program”, 23-30 July.
- CRYSTAL hands-on course “MSSC2016 – Ab-initio Modelling in Solid State Chemistry”, 19-23 September, Imperial College London
- 4th TYC Energy Materials Workshop 14-16th December 2016 - King's College London

CCPBioSim

Tom Keal lead a public discussion on future developments in QM/MM methods on day 2 of the 2nd CCP5/CCPBioSim Multiscale Modelling Conference (14th April).

A CCPBioSim tutorial workshop week was held at Bristol on 6-10 June covering a wide range of aspects of biomolecular modelling. A training workshop on FESetup was delivered by Hannes Loeffler on day 3 of the training week day (54 attendees).

Hannes Loeffler and Tom Keal gave talks at the November joint CCP5/CCPBioSim training workshop “Simulations for the Experimentalist and Industrialist” at Diamond (RAL), on the topics of classical and multiscale biomolecular simulation including showcases from the CCPBioSim community (26 attendees).

CCPmag

CCP-mag has co-sponsored and co-organized the KKR Hands-On course, which was held in Daresbury, 14-17 November 2016. The course was run as a joint training event between CCP-mag, CCP9 and the COST network EUSpec. Martin Lueders delivered 3 lectures on DFT and magnetism. The course was attended by 25 participants, of which 7 were from the UK.

Various discussions with electronic structure communities showed the common interest in common data formats. It was decided to merge some of these activities and to use CCP-mag support to further develop the ESCDF format and library. In this way, large parts of what already has been developed can be used for the magnetism community.

In November, the communities of CCP-mag, CCP9, and EUSpec (an EU initiative on spectroscopy) joint forces to organise a KKR Hands-On course, which has been held at Daresbury. Martin Lueders

delivered 3 lectures on density functional theory (DFT) and applications to magnetism. (24 participants form throughout Europe).

An advanced VAMPIRE hands-on course was held in York after the IoP Magnetism winter school. The course was organized by Richard Evans from York.

A hands-on course for the SpinW code, which is used by the neutron scattering community to simulate magnetic excitations was held in February at RAL.

Martin Lueders presented the collaborative work on magneto-caloric materials at the JEMS2016 conference.

CCP-NC

In August, the annual CASTEP workshop was held in Oxford, providing one week of training in the theory of DFT and the practical use of CASTEP to attendees from all over the world. Great attention was given as usual to ab-initio NMR calculations and related topics. Two seminars were held on account of CCP-NC by Simone Sturniolo – one focusing around the use of MagresView for post-processing of NMR CASTEP results and the other around the use of Python and Soprano for more complex tasks of random structure searching, with and without NMR reference data.

CCPQ

Training activities have been in the form of specialized group meetings and one-to-one interactions (local and virtual): these include SEG's tutorial meetings with QUB on RMT restructuring ('proper' modularization) and CCPForge, and with TNT on the Build Service and the Virtual Machine, MP's discussions with QUB on static inner region codes for double-continuum RMT, MP's meetings with AL (and JDG) on TIMEDELN, planning discussions for UKRMol+ and the possibilities for novel technology, and discussions with Aberdeen re interpretation of antihydrogen calculations.

CCPPlasma / HECPlasma

There were three presentations at BOUT++ workshops and meetings during this period, which were aimed at allowing code users to take advantage of new code features.

Joseph Parker provided two days of GS2 training for a PhD student, and one day of BOUT++ training to a CCFE user.

The GS2 performance analysis and the new collision operator implementation were documented, and will be presented at the GS2 developer meeting in Summer 2017.

Joseph Parker collaborated with Peter Hill (University of York) to produce a new website for the BOUT++ project (http://boutproject.github.io/)

CCPi

We have assisted via advertisement links, license management and show-and-tell sessions for seven training courses; mainly focussed on materials science visualisation.

- Sri Nagella hosted a full-day FEI Visit and Workshop at RAL (24 November 2016 - 12 attendees)
- Noriko Griffiths coordinated two Avizo courses in Manchester (13 October and 16-18 August, 20 places each); a Drishti workshop (13 June, 8 attendees); and a Training Session with Parmesh Gajjar on hacking the Nikon imaging devices (18 May, 7 attendees).
- Martin Turner assisted in some pre-ToScA Workshops on Monday 5th September 2016 at the University of Bath; provided by the three systems Avizo, VGStudio Max and Drishti (38 attendees) and gave a one hour session for the Hartree Summer School - Image Based Modelling examples (28 June , 12 attendees)

There have also been three main Public Engagement events over this period. The RCaH's Royal Society exhibit travelled to Manchester Science Festival as a satellite exhibition on 24-28 October 2016; at ESOF event - CCPi stand at the Great Hall in the Sackville Street Building and during the DL Open Week (5-9 July: a total of 815 people were given the "vis treatment").

CCPPetMR

Two major external one-day events were co-organised that incorporated training; a PETMR informal gathering on 7 September for those attending ISMRM-BC, at Leeds (Attendance 73 with 9 speakers) and a STIR Users' & Developers' Meeting on 3 November during the IEEE NSS-MIC (Attendance 47 with 6 speakers).

There has been one Public Engagement event with Manchester MRI. "Manchester Brain Box" linked together the scanning process with results available on a touchcreen presentation (https://mcrbrainbox.wordpress.com/) on 19 June. 90 people crawled through the 'pretend' MRI scanner and received a scanned image of 'their' brain.

Our main outreach activities during the reported period were our regular (every 6 weeks) Software Framework meetings, where we presented our development progress to - and got feedback from - our potential users from PET-MR research community (KCL, Leeds, Manchester and other Universities' researchers) and discussed data related issues with tomographic equipment industry representatives. The attendance is strong (the average is 20, with a maximum 24), comprising of attendees from a growing number of universities and the major imaging scanner manufacturers, includinge.g.including Siemens and, GE; and all continuing the an up-wards growing trend. Two trends are worth noting.: Firstly,1) a majority of the universities and companies attendinged our developers' meetings are funded independently funded, i.e. outside of the core CCP support, indicating a strong community commitment. Secondly,; and 2) we have already attracted independently funded university researchers who are now actively contributing to the testing and documentation of the codes, despite the early stage of the project. Average attendance of these meetings in the reported year was 20, maximal 24.

CCPPETMR has funding to support the exchange of researchers (staff and students) between institutions. Two exchange programs were supported this year: between UCL and University of Leeds and between UCL and Frederic Joliot Hospital at CEA, Orsay, France.

We also organized PET-MRI Image Reconstruction workshop at the 22nd Annual Scientific Meeting of the British Chapter of the ISMRM at Leeds University, 7-9 September 2016, and UCL PET/MRI Methodology Workshop, 21-23 September 2016. We have also supported, promoted and advertised the network within; the STIR User's and Developers Meeting (November 2016), two external seminars (University of Leeds, November 2016 and April 2017): and a Public Engagement stand at British Science Week for MRI datasets (University of Manchester, March 2017).

UK COMES

DL_SOFTWARE training workshop and Hack Day (18-20 April, UCL): DL_MESO present (along with other DL codes) with lectures and exercises to 20 attendees. Michael Seaton spent 3 days on training with an additional day on organisation.

PRACE Technical Training School, "Code Modernisation for Intel Multi Core and Xeon Phi Architectures" (25-28 April, National Center for Supercomputing Applications, Sofia, Bulgaria), lectures and code dungeon to 30 attendees. Michael Seaton gave a presentation on DL_MESO optimisation work ("Evolution and revolution: optimising mesoscale modelling codes for Intel Xeon Phi") and supplied DL_MESO_LBE code as an example code for code dungeon

CCP5 Summer School (11-20 July 2016, Lancaster) had 62 attendees. Michael Seaton spent a day on training in mesoscale modelling techniques.

CCP5 Simulations for the Experimentalist and the Industrialist (15-16 November 2016, ISIS) had 25 attendees. Michael Seaton gave a talk related to mesoscale modelling techniques and their application (“Mesoscale Dynamics”).

A DL_SOFTWARE training event took place at STFC Daresbury Laboratory on 5-7 December 2016 (25 participants).

HEC-BioSim

A training workshop on Longbow entitled “A Light Weight Tool for Automated Job Submission” was delivered as part of the CCPBioSim training week day 2. The theme of the training day was about how to go from setting up a single simulation through to high volume automated simulation and analysis (54 attendees).

A talk at a Daresbury technical forum lead to a request for a short hands on demonstration of Longbow. Three Hartree Center projects are now making use of Longbow as the job submission and management tool within their code, one of which is a simulation pipe-lining framework and the other two focused around automated compilation and runtime optimisation.

Appendix 5: Risks

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 development and novel architecture systems for evaluation and development 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

Planned Staff to Project Bookings

The following table shows the planned staff to project bookings for FY 2017/18 with changes from the report submitted in January 2017 highlighted yellow.

Project Office		FTE	Project Total
	M Forster	~~0.20~~ 0.05	
	S Miller	~~0.35~~ 0.00	
	D Jones	~~0.50~~ 0.70	
	V Kalavsky	0.50	
	M O'Sullivan	0.25	
	RIG Group	0.25	
	B Montanari	0.50	

			~~2.05~~ 2.25
CCP5			
	I Todorov	0.00	
	T Keal	~~0.08~~ 0.20	
	J Purton	0.79	
	C Yong	~~0.59~~ 0.31	
	M Seaton	0.10	
	I Scivetti	1.00	
	V Sokhan	1.00	
			~~3.56~~ 3.40
CCP9			
	L Petit	1.00	
	M Lueders	~~0.70~~ 0.20	
	J Jackson	1.00	
			~~2.70~~ 2.20
CCPmag			
	M Lueders	0.25	
	B Searle	0.15	
			0.40
CCPNC			
	S Sturniolo	1.00	
	A Bartok Partay	1.00	
			2.00
CCPQ			
	M Plummer	1.00	
	S Lamerton	~~0.36~~ 0.45	
	A Sunderland	0.50	
			~~1.86~~ 1.95
CCP Plasma			
	J Parker	0.80	
			0.80
CCPi			
	R Fowler	0.20	
	S Nagella	0.60	
	E Yang	0.10	
	E Pasca	0.60	
			1.50
CCPPetMR			
	E Pasca	0.40	
	E Ovtchinnikov	1.00	
	E Yang	0.10	
			1.50
CCP BioSim			
	H Loeffler	1.00	

	T Keal	0.20	
			1.20
MCC			
	L Bernasconi	1.00	
	I Todorov	0.75	
	T Keal	0.50	
	~~B Montanari~~ B Searle	~~0.25~~ 0.22	
			~~2.50~~ 2.47
UKCP			
	D Jochym	1.00	
			1.00
UK-COMES			
	M Seaton	0.45	
	J Meng	0.55	
			1.00
HEC Plasma			
	J Parker	0.20	
			0.20
HEC BioSim			
	J Gebbie	1.00	
			1.00
Software Outlook			
	L Mason	0.40	
	S Thorne	0.60	
	A Taylor	~~1.00~~ 0.79	
			~~2.00~~ 1.79


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


2016
2017
2018
2019
2020
2021
CCPi
E Ovtchinnikov
M Turner
R Fowler
S Nagella
E Yang
E Pasca
CCPPetMR
R Fowler
M Turner
E Pasca
E Ovtchinnikov
E Yang
CCP BioSim
H Loeffler
T Keal
MCC
C Yong
L Bernasconi
I Todorov
T Keal
B Montanari
B Searle
UKCP
D Jochym
P Byrne (Durham)
Additional Person
UK-COMES
M Seaton
J Meng
HEC Plasma
J Parker
HEC BioSim
J Gebbie
Additional Person
Software Outlook
M Ashworth
K Sivalingham
L Mason
S Thorne
A Taylor