EPSRC Service Level Agreement with STFC for Computational Science Support

FY 2018/19 Annual Report

(*Covering the period 1 April 2018 – 31 March 2019*)

TECHNICAL APPENDIX

May 2019

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CCP and HEC PLANS 2019/20 (1 April 2019 – 31 March 2020)

Rows in tables highlighted in yellow indicate a change from, or an addition to, the previous version of these plans submitted in the CoSeC Interim Report in December 2018.

Project Office	Milestone	Target Date
	Attend CCP and HEC committee meetings as required	Ongoing
	Support CCP and HEC conferences and workshops as required	Ongoing
	Respond to recommendations from the SLA Review 2018	Ongoing
	Carry out outreach activities (social media, brochures, talks)	Ongoing
	Maintain and update CoSeC web site	Ongoing
	Regular meetings with Technopolis to discuss conclusions from the impact report	Ongoing
	Weekly internal STFC meeting to discuss progress with all CoSeC activities	Ongoing
	Work with Technopolis to complete CoSeC impact report	Q2 2019
	Arrange internal project meetings with funded CCPs and HECs – April 2019 – individual meetings	Q2 2019
	Prepare and submit annual CoSeC SLA report – June 2019	Q2 2019
	Arrange and attend the CCP Steering Panel June meeting	Q2 2019
	Attend the CoSeC SLA Steering Committee July meeting	Q2 2019
	Arrange internal project meetings with funded CCPs and HECs – July 2019 – DL / RAL site meetings	Q3 2019
	Compile and submit ARCHER renewal proposal	Q3 2019
	Prepare and submit interim CoSeC SLA report – December 2019	Q4 2019
	Arrange internal project meetings with funded CCPs and HECs – October 2019 – individual meetings	Q4 2019
	Arrange and attend the CCP Steering Panel December meeting	Q4 2019
	Attend the CoSeC SLA Steering Committee December meeting	Q4 2019
	Arrange internal project meetings with funded CCPs and HECs – January 2020 – DL / RAL site meetings	Q1 2020

FY 19/20 Staffing	Effort
Damian Jones	0.70 FTE
Dawn Geatches	0.20 FTE
Barbara Montanari	0.25 FTE

Gilberto Teobaldi	0.15 FTE
RIG Group	0.20 FTE
Total	**1.50 FTE**

CCP5	Milestone	Target Date
Training & Outreach	Day to day maintenance of the website	Ongoing
	Workshops	Ongoing
	Committee elections	Q2 2019
	DL_Software Training	Q2 2019
	CCP5/CCPBioSim School, Chile	Q2 2019
	Introduction to Modern Fortran	Q2 2019
	CCP5 Summer School	Q2 2019
	CCP5 bursaries programme	Q2 2019
	CCP5 Outreach Competition	Q2 2019
	CCP5 AGM	Q3 2019
	DL_Software Training	Q4 2019
	Potentials cross CCP5 – international	Q1 2020
	DL_Software Training	Q1 2020
Chemshell	Support for Z-matrices for automated forcefield parameterisation	Q2 2019
	Development of an ADF interface in Py-ChemShell	Q3 2019
	~~Creation of Jupyter notebook versions of the Py-ChemShell tutorials~~ Completion of Aten GUI plugin	~~Q1 2020~~ Q3 2019
	New python-based testing system	Q4 2019
	Release of Py-ChemShell ~~2019~~ 2020	~~Q2 2019~~ Q1 2020
DL_Monte	Set up automated testing methods on GitLab	Q2 2019
	DL_MONTE project to new GitLab service provided by CoSeC	Q4 2019
	Provide new download mechanism for DL_MONTE	Q4 2019
DL_POLY_4	Thermal conductivity EMD	Q2 2019
	Export dlpoly files from gulp	Q2 2019
	Release 4.10	Q2 2019

	Implementation of the EVB method within DL-POLY	Q2 2019
	Development and implementation of Shapes for isobaric conditions	Q2 2019
	Simple gui to generate control	Q3 2019
	Simple gui for visualising statis	Q3 2019
	Extending DL_POLY to include chemically bonded atomic/shapes mixtures as a general framework for coarse-graining biomolecules	Q3 2019
	Python interface	Q3 2019
	Two states EVB alpha release	Q3 2019
	Generalised GB beta release	Q3 2019
	Demonstrator application using the developed framework leading to a journal publication	Q4 2019
	Restrained MD	Q4 2019
	Hybrid Monte Carlo	Q4 2019
	Add short range potentials from gulp to dlpoly 4 for interoperability	Q4 2019
	EVB proof of concept application	Q4 2019
	Generalised GB alpha release	Q4 2019
	Test and validate the implementation of Shapes in DL_POLY in the canonical ensemble for all cases: ellipsoid of revolution, biaxial ellipsoids including loaded and skewed cases	Q4 2019
	Move tutorials to new infrastructure trialed at recent training	Q1 2020
DL_ANALYSER/DL_FIELD	Implement OpenMP features in DL_ANALYSER, to speed up analysis processes, especially for larger models. In the first instance, allow concurrent analysis to be carried out over various Analysis Components.	Q2 2019
	Release of DL_FIELD version 4.4 (testing + manual updates)	Q2 2019
	Maintenance and implementation of existing and new force field schemes: Inclusion of new force fields such as Amber GAFF, OPLS for ionic liquids	Q3 2019
	Release of DL_ANALYSER version 2.2	Q4 2019
	Automation of solvation for multiple potential models, including inorganic models	Q4 2019
	Release of DL_FIELD version 4.5 (testing + manual updates)	Q1 2020
DL_MESO	Implementation of PPPM electrostatics in DL_MESO	Q3 2019
	Implementation of fixed-length constraints	Q3 2019

	Bond-crossing prevention algorithms in DL_MESO	Q1 2020

FY 19/20 Staffing	Effort
John Purton	~~0.45~~ 0.38 FTE
Ilian Todorov	~~0.20~~ 0.63 FTE
~~Chin Yong~~ Andrey Brukhno	~~0.51~~ 0.50 FTE
Michael Seaton	~~0.07~~ 0.32 FTE
You Lu	~~0.20~~ 0.50 FTE
Vlad Sokhan	1.00 FTE
Ivan Scivetti	1.00 FTE
Alin Elena	~~0.68~~ 0.05 FTE
Total	**~~4.11~~ 4.38 FTE**

CCP9	Milestone	Target Date
	Paper on Gd-intermetallic alloys	Q2 2019
	3rd Daresbury Questaal school	Q2 2019
	Review paper Computer Physics Communications	Q2 2019
	SuperSTEM collaboration: EELS modelling with GW and BSE (resubmit proposal)	Q2 2019
	Results on various SIC calculations with LMTO-ASA code	Q3 2019
	OpenMP implementation in Crystal code: two-electron forces	Q3 2019
	Cristal field collaboration with Salford	Q3 2019
	Validation & verification lanthanides	Q3 2019
	~~Questaal Optimization and load balancing~~	~~Q3 2019~~
	Submit Paper on Eu2In	Q3 2019
	Submit paper on helical ordering in Mn_3Sn	Q3 2019
	Submit paper on incommensurate ordering in CrB_2	Q4 2019
	Study twin defects in NiO with Hutspot/DLM	Q1 2020
	OpenMP implementation in Crystal code: DFT forces	Q1 2020
	Implementation of SIC in LMF; deployment phase	Q1 2020

Staffing	Effort
Leon Petit	1.00 FTE
~~Martin Lueders~~	~~0.28 FTE~~
Jerome Jackson	1.00 FTE
Barry Searle	~~0.60~~ 0.70 FTE
Total	**~~2.88~~ 2.70 FTE**

CCPmag	Milestone	Target Date
	~~ESCDF: testing suite finished and magnetic data implemented (M. Lueders)~~	~~Q2 2019~~
	Magnetic exchange interactions implemented in Quantum Espresso (K. Cao)	Q2 2019
	Paper on theory-experiment comparison of Fe data submitted (Lueders, Cao)	Q2 2019
	Organization of computational magnetism session at Magnetism 2019	Q2 2019
	Calculation of the magnetic susceptibility of Pd (K. Cao)	Q3 2019
	~~Initial investigations for using the vertex functions, developed by B. Cunningham (Belfast) for the magnetic susceptibility (Lueders)~~	~~Q4 2019 – Q1 2020~~
	Liaise with P. Hasnip to implement the exchange couplings in CASTEP (K. Cao)	Q4 2019
	Liaise with Keith Refson to implement TDDFT for spin fluctuations in CASTEP (K. Cao)	Q4 2019 – Q1 2020

Staffing	Effort
~~Martin Lueders~~ New Hire	0.22 FTE
Kun Cao	~~1.00~~ 0.50 FTE
Total	**~~1.22~~ 0.72 FTE**

CCPNC	Milestone	Target Date
	Maintenance and improvement of the Soprano library	Ongoing
	Development of new methods for the treatment of nuclear quantum effects in NMR	Ongoing
	Deployment of the CCP-NC database user front end for public use	Q2 2019
	Paper to be published on the technical details and benchmarks of meta-GGA functionals in planewave-pseudopotential packages	Q2 2019
	Implementation of the latest meta-GGA exchange-correlation functionals in CASTEP, and release for general use	Q2 2019
	Development of a new WebGL native molecular and crystalline structure visualiser to replace JMol at the core of MagresView.	Q3 2019
	Paper to be published on the Tran-Blaha method in planewave-pseudopotential packages	Q4 2019

	Development of a revamped MagresView using the new WebGL app as well as a renewed interface, modern JS technologies and testing pipelines for improved maintainability.	Q1 2020
	Automated generation of coefficients for dispersion-correction schemes, commensurate with exchange-correlation functionals	Q1 2020
	Combined Tight-Binding and Machine Learning model of aromaticity in hydrocarbon and amorphous carbon structures, to quantitatively determine Nuclear Independent Chemical Shifts	Q1 2020

Staffing	**Effort Funded**
Simone Sturniolo	~~0.99~~ 0.22 FTE
Albert Bartok-Partay	~~0.60~~ 0.42 FTE
Total	**~~1.59~~ 0.64 FTE**

CCPQ	**Milestone**	**Target Date**
Atomic R-matrix (and RMT)	Martin Plummer (MP): following CPC submission, perform any relevant changes according to referee reports.	~~Q2 2019~~ Q2 – Q3 2019
	Continued test calculations with feedback to QUB. Work with QUB people to allow them to use the code (with appropriate UK-AMOR proposals and time) for scientific work. Consider test cases for field-free intermediate energy scattering.	Ongoing (Q4 2019 – Q1 2020 for field-free work)
	Preparation for presentation possibilities at ICPEAC 2019 and satellites.	Q2 2019 (Q3 2019 for attendance if possible)
RMT	Andy Sunderland (AGS) continued work as required on GPU-BLAS and/or flexible parallelization. Review and decision on future work for the rest of the year, eg inner region task assignment (to be confirmed). [Priority for updating milestone in early Q3]	Q2 – Q3 2019
	Software Engineering Group (SEG): work with developers to allow large-scale highly parallel test cases to run with ANVIL: this may involve use of a forthcoming ARCHER(2) version of ANVIL.	Ongoing
	MP to continue discussions on possible ALC 'digital assets' funding and put in proposal if appropriate. MP to assist with or possibly join QUB double-continuum EPSRC proposal.	Q2 – Q3 2019
UKRMol(+)	AGS continued work as required on diagonalizers (see 2018-19 plans). Review and decision on future work for the rest of the year. Specific milestone: related to diagonalizers; find a practical workaround to limits the SLEPC library places on the number of eigenvalues that can be calculated due to memory allocation within SLEPC (either by efficient 'underpopulation' of nodes or by	~~Q2 – Q3 2019~~ Q3 2019

	batched calculation of groups of eigenvalues via spectral transformations).	
	Completion of memory optimization merge and final test case. Assist UKRmol+ users with any queries related to memory optimization. Possible submission to ICPEAC satellite POSMOL conference.	Ongoing (Q2 2019 for completion and POSMOL)
	SEG: monitoring and assistance with R-matrix ANVIL project (details tbc) and other projects as decided in Q4 2018 meeting.	Ongoing
RMAT_REACT and PFARM	MP to oversee AGS's UK-AMOR work on parallel resonance and bound state determination (all year as UK-AMOR was allocated 0.2FTE for AGS)	Ongoing
	MP to work with the UCL group on any further expansion of PFARM functionality and theory papers or conference presentations.	Q2 – Q3 2019
	Ongoing maintenance of GPU-PFARM, opportunities for further PRACE funding. AGS: Follow-up work on PFARM/PSTGF comparisons as workload allows.	Ongoing (Q2 – Q3 2019 tbc)
TNT and QUANTICS	Continued Quantics porting and parallel testing and benchmarking, discuss appropriate new work for rest of year with G Worth. MP and SEG to agree support for QUANTICS-based ECAM workshop in July: SEG to provide a talk/course on ANVIL.	Q2 – Q3 2019
	SEG: Monitoring of TNT repository issues following move from CCPFORGE, continued work on PYTHON interface as needed. Further development work to be discussed with M Lubasch and TNT leaders (encourage further input and requests from university colleagues.	Q2 – Q3 2019
	Monitoring of ANVIL projects transferred from SESC Build Service	Ongoing
Antimatter	MP: Support as required for MML and/or D Green (following December 2018 discussions).	Ongoing
	MP: possible revival of studies of Kohn variational method theory and Ps- formation in 2nd half of year if double continuum work goes 'smoothly' following 2018-19 effort.	Q4 2019 – Q1 2020
General	MP: general support for webpages, general support and admin for the R-matrix GitLab site, admin duties as part of the UK-AMOR steering group as they arise.	Ongoing
	MP (and AGS, SEG): look out for further funding opportunities (in addition to those above). In particular, be prepared for the CCP renewal Call and assistance with relevant parts of the proposal. Follow-up work on possible CCPQ/UK-AMOR/CCP-PLASMA networking and/or meeting.	Ongoing
	SEG: general practical advice with repositories, best practice, ANVIL use.	Ongoing

Staffing	Effort
Martin Plummer	1.00 FTE
SEG	0.40 FTE
Andrew Sunderland	0.60 FTE
Total	**2.00 FTE**

Plasma	Milestone	Target Date
	BOUT++: Assess the available kinetic neutrals codes and atomic/molecular databases. Couple the most appropriate to BOUT++ to allow Monte-Carlo modelling of neutral gases.	Q2 2019
	GS2: Assess and rationalize the communication in GS2's implicit field solve. Distinguish between communication required for the field solve, and communication only required by diagnostics, to minimize calls to expensive broadcast functions.	Q3 2019
	BOUT++: Improve BOUT++'s handling of complex geometries to allow composable domains, more complicated branch cuts, and non-periodic Z-domains.	Q4 2019
	GS2: Implement unit testing framework for in GS2. Couple testing to continuous integration service Anvil to provide automated testing of PRs. Also couple tests to code coverage tracking service.	Q1 2020

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

CCPi	Milestone	Target Date
	Website, mailing lists, source code and data archives	Ongoing
	Organise exec committee and working group meetings, as well as monthly show-and-tell sessions	Ongoing
	Support current training courses and organise developer workshops. Assist in new proposal writing.	Ongoing
	Working with CCPi Flagship team in improving Core Imaging Library (CIL) and integrating the codes from flagship into CIL.	Ongoing
	Embed CCPi software into DAaS virtual machine to allow facilities users (DLS, ISIS) to perform analysis on their datasets from remote	Ongoing
	Collaboration: Working with Brian Bay (USA) on improving the digital volume correlation codes and distributing it to CCPi community.	Ongoing

	Case Studies: Three case studies will be undertaken with ISIS/Diamond and Universities	Ongoing
	Code sharing with CCPPETMR	Ongoing
	Release updated version of Simpleflex segmentation algorithm developed together with Hamish Carr (Leeds) and his student. Distribute and collaborate with Diamond i12 staff to test the segmentation on real data.	Q2 2019
	Help to organise the main ToScA conference; September 2019	Q3 2019
	Embed lab based framework: UoM/ UoS/ UoW	Q3 2019

Staffing	**Effort**
Edoardo Pasca	0.56 FTE
~~New Hire~~ Gemma Fardell	1.00 FTE
Total	**1.56 FTE**

CCP PET-MR	**Milestone**	**Target Date**
	Manage CCP PET-MR website, mailing lists and data archives for both simulated and acquired data.	Ongoing
	Organise exec committee, working group meetings, developers' days and other events.	Ongoing
	Support current training courses.	Ongoing
	Assist in new proposal writing.	Ongoing
	Visit sites in the network to gain experience with a few selected packages for image reconstruction and to get others started with SIRF	Ongoing
	Run continuous build and test system. Enable testing on ANVIL.	Ongoing
	Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide	Ongoing
	Optional: Profiling (and possibly speed-up) of PET reconstruction.	Ongoing
	SIRF Release 2.0	Q2 2019
	MR reconstruction with PET prior.	Q2 2019
	Joint motion estimation.	Q2 2019
	Finalise nonTOF support for GE PETMR scanners	~~Q1 2019~~ Q3 2019
	Optional: Investigate use of SWIG to create interface between c++ and target languages	~~Q2 2019~~ Q4 2019

	~~Motion-guided reconstruction~~ TOF support (no scatter)	~~Q3 2019~~ Q4 2019
	~~Joint PET-MR reconstruction using MATLAB or Python tools/toolboxes~~ SIRF Release 3.0	~~Q3 2019~~ Q4 2019
	~~SIRF Release 3.0~~ PET dynamics and gated (separate reconstructions)	Q4 2019
	List mode reconstruction without conversion to sinograms.	Q4 2019
	TOF support	Q1 2020
	Documentation on developing new functionality and interfaces	Q1 2020
	Support for more MR sequences (sequences to be determined)	Q1 2020
	~~Optional: GPU support~~ Motion guided reconstruction	Q1 2020
	Optional: ~~integration of other reconstruction packages into SIRF~~ Joint PETMR reconstruction using MATLAB or Python tools/toolboxes	Q1 2020
	SIRF Release 4.0	Q1 2020

Staffing	**Effort**
Evgueni Ovtchinnikov	1.00 FTE
Edoardo Pasca	0.30 FTE
Total	**1.30 FTE**

CCPBioSim	**Milestone**	**Target Date**
	Add modules to the online training and lead/support workshops	Ongoing
	FESetup – improve user documentation, installation and the management of dependencies	Q2 2019
	Joint project with CCP-EM/CCP4 - MD analysis to improve structure refinements.	Q3 2019
	FESetup – add integration with LOMAP for automating the creation of morph pairs lists	Q4 2019
	Multiscale workflows – test cytochrome P450 benchmarks with Tcl-ChemShell (and Py-ChemShell if available) and integrate into full CG,AA,QM/MM workflow	Q4 2019
	Reproduction of the membrane-bound protein multiscale modelling workflow from the first CCPBioSim software flagship project	Q4 2019

	~~Develop~~ Test BioSimSpace metadynamics node for binding kinetics calculations	Q1 2020
	~~Lead~~ Support organisation of the 4th CCPBioSim/CCP5 Multiscale Modelling Conference	Q1 2020

Staffing	Effort Funded
Sarah Fegan	1.00 FTE
Thomas Keal	~~0.20~~ 0.10 FTE
Kakali Sen	0.20 FTE
Sebastian Metz	0.10 FTE
Total	**~~1.20~~ 1.40 FTE**

MCC	Milestone	Target Date
CRYSTAL (subject to recruitment)	Organise/attend monthly meetings of UK CRYSTAL developer at RAL, Oxford or Imperial College.	Ongoing
	Supervision of Dr N Holzmann concerning two projects with CLF and ISIS.	Ongoing
	MSSC2019 Summer School, Imperial College London	Q3 2019
	Fixing some issues with the parallel (Pcrystal) version of the TD-DFT module in the interface routines with the CP-HF code.	Q3 2019
	Refactor of massively parallel (MPP) extension	Q1 2020
	Development of training material	Q1 2020
SAINT	Assist MCC PDRA with generation of symmetrised surface models from bulk unit cells for backend software	Q3 2019
	Assist on generation of inputs to enable backend software to run CRYSTAL simulations	Q1 2020
ChemShell/DL-FIND	Supervision of ChemShell work package in MCC “SAINT” software flagship project	Ongoing
	Maintain ChemShell on ARCHER and Tier 2 systems (e.g. Thomas)	Ongoing
	Extend the interface to LSDalton to support embedded cluster QM/MM calculations (dependent on ECP implementation by the Dalton developers)	Q3 2019
	~~Implement a framework for multiple electronic state QM/MM calculations and interface to DL-FIND for conical intersection optimisations.~~ Interface ChemShell to DL_MONTE	Q1 2020
DL_POLY	International training in Chile planned in May.	Q2 2019

	Refactoring work, supervision and reporting.	Q3 2019
	~~Collaboration (two temperature model, Zeolites, etc)~~	~~Q1 2020~~
~~**DL_FIELD**~~	~~Testing of multiple-potential capabilities.~~	~~Q2 2019~~
	~~Conversion to Amber's topology file.~~	~~Q1 2020~~
	~~Zeolite forcefield model~~	~~Q3 2019~~

Staffing	**Effort**
TBC (CRYSTAL)	0.80 FTE
Barry Searle (SAINT)	0.20 FTE
Ilian Todorov (DL_POLY)	~~0.30~~ 0.10 FTE
~~Chin Yong (DL_FIELD)~~	~~0.30 FTE~~
Tom Keal (ChemShell)	~~0.10~~ 0.05 FTE
~~David Gunn (ChemShell)~~	~~0.30 FTE~~
John Purton	0.30 FTE
Total	~~**2.00**~~ **1.45 FTE**

UKCP	**Milestone**	**Target Date**
	Continued consolidation of Raman and NLO code, including user tutorial material.	Q2 2019
	Paper to be published on the technical details and benchmarks of meta-GGA functionals in planewave-pseudopotential packages	Q2 2019
	Implement van der Waals DFT (Dion) functional in CASTEP.	Q2 2019
	Extension of Raman/NLO code for phonon lifetimes to be applied in Bolzmann Transport Equations.	Q2 2019
	Prepare and release existing Genetic Algorithm CASTEP tool, including portability and application case study.	Q2 2019
	Bring electronic licensing system for academic CASTEP into production.	Q3 2019
	Co-organization and teaching of CASTEP workshops (both user and code development) in Oxford.	Q3 2019
	Prototype interface for CASTEP to the YAMBO code.	Q3 2019
	Release management of CASTEP v20.1 including documentation and liaison with major HPC services.	Q4 2019
	Organisation of 2019 CASTEP "codefest" core developer workshop.	Q4 2019
	Automated generation of coefficients for dispersion-correction schemes, commensurate with exchange-correlation functionals	Q1 2020

Staffing	Effort
Dominik Jochym	0.80 FTE
Albert Bartok-Partay	~~0.20~~ 0.10 FTE
Total	**~~1.00~~ 0.90 FTE**

UKCOMES	Milestone	Target Date
	Immersed boundary methods in DL_MESO	Q2 2019
	Implement LES turbulence model in MPLB code	Q3 2019
	High density contrast Lishchuk algorithm for multiple fluid systems	Q3 2019
	Viscoelastic rheological models in DL_MESO	Q4 2019
	Implement ray-tracing algorithm for two-dimensional polygons	Q1 2020

Staffing	Effort
Michael Seaton	0.30 FTE
Jianping Meng	0.30 FTE
Total	**0.60 FTE**

HECBioSim	Milestone	Target Date
	Update and maintain website	Ongoing
	JADE and ARCHER benchmarks to be kept up to date	Ongoing
	Support HECBioSim users of JADE by compiling software and monitor usage, create user accounts and manage allocations.	Ongoing
	Create best practice guides for ARCHER and JADE for biosimulation users	Q2 2019
	Complete the Release of Longbow V1.5.3	Q2 2019
	Jupyter project with Charlie Laughton (Nottingham)	~~Q2 2019~~ Q3 2019
	Entropy project depending on committee feedback (provisional based on acceptance of proposal currently being worked on Q3)	~~Q3 2019~~ Q4 2019
	Complete the Kubernetes infrastructure deployment on Oracle Cloud for the CCPBioSim training Platform (Date not yet set due to procurement delays).	Date not yet confirmed
	Work with Syma Khalid to develop a training resource for Longbow as part of a collaboration with BioExcel	Date not yet confirmed

Staffing	Effort

James Gebbie-Rayet	1.00 FTE
Total	**1.00 FTE**

UKAMOR	**Milestone**	**Target Date**
	Attend UK-AMOR management committee meetings as required and follow up accordingly.	Ongoing
	Finalize incorporation of PFARM into the TIMEDELn resonance package multi-level parallel framework and make significant progress on the incorporation of bound states (and if time allows RESON) into the framework. With the concerns raised about the numerical instability of parts of the existing bound state code, the actual progress will depend on testing how this affects the new code and how much it can be avoided using PFARM technology. The bound state package is the priority. If time allows and RESON has been also been incorporated, MP and AGS to decide on feasibility of including 'S-matrix' pole searches in consultation with J Tennyson.	Q2 2019 – Q1 2020
	Follow up any opportunities for relative benchmarking of PFARM and complementary UK-AMOR code PSTGF using PRACE funding if possible. This is dependent on the results of the work and discussion in Q1 2019, and if time and the limited FTE allows.	Q2 – Q4 2019
	Review of progress on resonance package work, new/revised milestones for Andrew Sunderland 2019-2020 (and decisions on the nature of 2020-2021 support)	At least quarterly

Staffing	**Effort**
A Sunderland	~~0.20~~ 0.30 FTE
Total	**~~0.20~~ 0.30 FTE**

UKTC	**Milestone**	**Target Date**
	Extend benchmark study of the Taylor-Green vortex test case to the turbulent flow regime using LES within Code_Saturne	Q3 2019
	Investigate development of a scalable Lagrangian particle tracking capability	Q1 2020

Staffing	**Effort**
X Gu	0.40 FTE
Total	**0.40 FTE**

UKCTRF	Milestone	Target Date
	On-going validation and testing of HAMISH throughout its development	Ongoing
	Continued code-modernisation of HAMISH	Q3 2019
	Development of adaptive meshing capability for HAMISH (sequential)	Q4 2019
	Research and develop parallel adaptive meshing strategy for HAMISH	Q1 2020

Staffing	Effort
J Fang	0.50 FTE
Total	**0.50 FTE**

Software Outlook	Milestone	Target Date
Hybrid Programming: CPU+GPU	Initial comparative study for the frameworks considered. Benchmark runs have been performed. Results need turning into technical report and training course	Q2 2019
	Hackathon training organised jointly with Sheffield University's RSE Group	Q3 2019
	Comparative study using example CCP/HEC codes	Q4 2019
	Work package report and recommendations	Q1 2020
Physics and Maths Libraries	Audit of CCP/HEC codes to identify target 3D problems requiring the use of improved linear algebra libraries	Q2 2019
	FFT: comparative study. Delayed due to staff illness. Benchmark runs have been performed. Results need turning into technical reports	Q2 2019
	Identification of suitable candidate libraries: provide their attributes on the Software Outlook website	Q2 2019
	Comparative study	Q4 2019
	Work package report and recommendations	Q4 2019
	Linear Solvers: survey appropriate solvers for use in EPOC, BOUT++ and other applicable codes. BOUT++ work started but the FFT work was prioritised and this was put on hold until 19/20	Q4 2019
Code Coupling at Scale	Audit of available code coupling tools and of proposed coupling activities in the community.	Q3 2019

	Implementation of coupling tools within a series of test cases from a range of applications**. (Note: milestone is after 31 March 2019 but work starts in 2019/20)**	Q2 2020
	Instrumentation of coupled cases with a profiler and acquisition of profiling data for each. **(Note: milestone is after 31 March 2019 but work starts in 2019/20)**	Q2 2020
	~~Work package report with findings and recommendations. (Note: milestone is after 31 March 2019)~~	~~Q3 2020~~
General Consultancy	Deliver work (agreed with Working Group) in a timely manner	Q1 2020

Staffing	**Effort**
~~Luke Mason~~	~~0.20 FTE~~
Sue Thorne	0.60 FTE
~~Andrew Taylor~~	~~0.20 FTE~~
Aidan Chalk	0.40 FTE
Philippe Gambron	0.50 FTE
Total	**1.50 FTE**

HIGHLIGHT PAPERS

CCP5	Reorganization energy upon charging a single molecule on an insulator measured by atomic force microscopy. Shadi Fatayer, Bruno Schuler, Wolfram Steurer, Ivan Scivetti, Jascha Repp, Leo Gross, Mats Persson & Gerhard Meyer, Nature Nanotechnologyvolume 13, pages376–380 (2018)
CCP9	Magnetic excitations in non-collinear antiferromagnetic Weyl semimetal Mn3Sn, P. Park, J. Oh, K. Uhlířová, J. Jackson, A. Deák, L. Szunyogh, K. H. Lee, H. Cho, H. L. Kim, H. C. Walker, D. Adroja, V. Sechovský & J. -G Park, npj Quantum Materials volume 3, Article number: 63 (2018)
CCP-NC	Simone Sturniolo, "Computational applications of the many-interacting-worlds interpretation of quantum mechanics", Phys. Rev. E 97, 053311
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CCPi	Daniil Kazantsev, Valery Pickalov, Srikanth Nagella, Edoardo Pasca, Philip J. Withers TomoPhantom, a software package to generate 2D–4D analytical phantoms for CT image reconstruction algorithm benchmarks. SoftwareX, Volume 7, January–June 2018, Pages 150-155
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MAJOR CODE DEVELOPMENTS

CCP5	**DL_POLY_4**	Version 4.09 was released in September 2018. • New features, functionality, (re)implementations, etc. • modified morse • Ziegler-Biersack-Littmark, ZBL, ZBL mixed with Morse and Buckingham • Mei-Devenport-Fernando taper for Lennard-Jones, 12-6 and Buckingham • Rydberg • modified LJ • new RDF error bars calculation functionality • new optional I/O file-naming functionality • CONTROL file can be passed as command line argument under any name • main input/output filenames can be changed via directives in CONTROL file • two-temperature model (TTM) • electronic temperature evolution for metal and non-metal systems • initial electronic energy depositions for lasers and Swift heavy ion irradiation • inhomogeneous Langevin thermostat (also available without TTM) • new umbrella sampling restraint external field nd RDFs • bug release: November 2019 4.09.01 • bug release: January 2019 4.09.02
	DL_POLY_4	Complete refactoring of DL_POLY_4: • all routines are in a module • there is no data stored in module anymore • testing vastly improved from 30 to 170 tests • parts of code rewritten to simplify • removed leapfrog features • various bug fixes • ci infrastructure updated to be in line with the new developments. • added new API documentation system FORD

	DL_FIELD	Version 4.3 release
	DL_MESO	• Added bounceback reflection for hard surfaces and frozen bead walls (no-slip boundary condition) • Several bug fixes to DPD code in preparation for imminent release
	Chemshell	• New tutorial pages based on Sphinx • A new test system • An example Jupyter notebook • Release of Py-ChemShell 2019
	DL_MONTE	Library of user cases extension ongoing

CCP9	**Questaal**	The HDF5 implementation developed during the previous ECSE has been ported to the current version of the code
	DLV	Maintenance performed
	CRYSTAL	Successful OpenMP implementation of the electron-nucleus interaction almost doubling of the performance for two threads

CCP-mag	**ESCDF**	New library structure implemented

CCP-NC	**Soprano**	• New functionality for saving of structure collections as folders with associated metadata • Asymmetric unit cell reduction for comparison between defect sites in symmetric structures • Support of sklearn for clustering and introduction of some clustering comparison metrics (confusion matrix, Fowles-Mallows index)
	CCPNC Database	• Added option of multi-file uploading with a compressed archive • Added a JavaScript and Python test suite • Added search functions by stochiometry and molecular composition
	crystcif-parse	• Developed parsing of the CIF data format according to 1.1 specification • Developed basic parsing of key atomistic structure properties (unit cell, atomic positions and species)

	meta-GGA	• Consistent pseudopotentials • Analytic first derivatives to enable geometry optimisations and molecular dynamics
	crystvis-js	3D rendering for atoms, bonds, and other core elements of crystal visualisation using Three.js
	pymuon-suite	• Random generation of hydrogen defect structures • Unperturbed Electrostatic Potential • Nuclear independent hyperfine tensors • Quantum harmonic vibrational averaging
	pynics	• Python version of the current2nics tool to compute nuclear independent chemical shieldings • Compute buildup functions for chemical shieldings (as seen in the recent paper “The Lorentz sphere visualized”)

CCPQ	**UKRMol(+)**	Memory optimization of molecular orbital re-indexing transformations and detailed testing of ‘exact’ reproducibility of integral results *Substantial gains (eg memory use 1/13 that of the original code for a test case): detailed debugging carried out: ‘exact’ reproducibility (to be) achieved in Q4 (ie October 2018)*
	PFARM (functionality)	• Adaptation for ‘heavy’ collisions and extension of range of outer region interaction potentials • Adaptation for multichannel potentials and correct space-fixed frame. *Heavy’ collision version included with the developing UCL RMAT_REACT suite, further developments will ‘keep step’ with this suite.Multichannel work initiated and testing begun (to be completed Q2 2019)*
	Double continuum atomic R-matrix code	Re-use of N-electron integrals for (N+1)- and then (N+2)-electron integrals. Restructuring of higher-level control modules to allow smooth progress from N -> N+1 -> N+2 electrons and associated partial merging of the ANG and HAM codes to minimize intermediate large data write-out. *Major computational bottleneck on integral evaluation overcome by careful sums over already computed integrals using ‘surfacing coefficient’ theory. Major intermediate data bottleneck adjustment to be completed Q2 2019.*

	All codes (R-Matrix, TNT, Quantics)	Assist with (to various extents) or perform transfer from CCPForge to GitLab (QUB for R-matrix, Oxford for TNT, UCL for Quantics.
	Quantics, TNT, RMT	• Set up codes on ANVIL with links to the relevant GitLab repositories. • Test new QUANTICS parallelism deployment on SCD cloud VMs. *Complete for Quantics, TNT. Particular aspects of RMT set-up (for certain large size meaningful test cases) being double-checked (into Q2 2019).*

CCPPlasma / HECPlasma	**BOUT++**	• Release of BOUT++ v4.2.0 • Further refinement of looping method included in v4.2.0 • Bugfix releases v4.2.1 and v4.2.2 *Significant feature release, details:* *https://github.com/boutproject/BOUT-dev/releases/tag/v4.2.0* *https://github.com/boutproject/BOUT-dev/releases/tag/v4.2.1* *https://github.com/boutproject/BOUT-dev/releases/tag/v4.2.2*
	GS2	• Release of GS2 v8.0 • Major overhaul of working practices • Feature/bugfix release v8.0.1 • Added CI using STFC's Anvil Jenkins server • Added coverage metrics with codecov • Improved documentation with FORD • Performance improved with better default options *Community moved from Sourceforge + svn to Bitbucket + git. Adopted "gitflow" workflow with protected branches, code review and CI. v8.0 is snapshot release at time of migration; releases v8.0.1 (bugfixes) and v8.1 (features) scheduled for next reporting cycle. https://bitbucket.org/gyrokinetics/gs2/pull-requests/46/gs2-v801-rc/diff. Project now citable: https://zenodo.org/record/2551067*

CCPi	**CCPi-PreProcessing**	No ongoing development

	CCPi-Recostruction	No ongoing development
	CCPi-Quantification	No ongoing development
	CCPi-Simpleflex	• Addition of different measures in the simplification of the Contour Tree • Creation of GUI
	CILViewer	• 2D and 3D viewer • Linking viewers • Selection box, line profile • GUI integration • Other development
	CCPi-Regularisation-Toolbox	• 7 regularisation algorithms for multithreaded CPU and GPU • MATLAB and Python interfaces • Further developments
	TomoPhantom	Initial working release
	CCPi-DVC	• Initial wrapping of code from Brian Bay • Code optimisation • DVC configurator Graphical User Interface • Development of parallel execution

CCP PETMR	**SIRF**	• Add advanced features Appendix to User Guide • Add more real data functionality (scattering etc.) • Add more documentation, including inline doxygen documentation in C++ sources and SIRF Developer Guide. • Implement PLS Prior • Implement 2D Filtered Back Projection • Introduce checks for Gadgetron crash • Create namespace sirf • Implement sorting of MR images • Implement unified data containers hierarchy in C++, Python and Matlab. • Implement common PET/MR image data hierarchy in C++, Python and Matlab. • Adapt SIRF for CIL compatibility • Prepare Release 2.0

CCPBioSim	**FESetup**	• Support for Amber18 • Bug fix for user defined parameters

MCC	**CRYSTAL**	• Hybrid OpenMPI/MPI parallelisation of one-and two-electron integrals. • Development of a general model of radiation damage in proteins based in TD-DFT calculations.
	ChemShell	• Interface to the QM code ORCA in Py-ChemShell • Support for embedded cluster QM/MM calculations with ORCA • Py-ChemShell ported to the ARCHER and THOMAS platforms • First Py-ChemShell beta release (v19.0) *Complete, with a paper accepted for publication*
	DL_POLY	• Refactoring work, supervision and reporting • Lectures for CCP5 Columbia (CCPBioSim/UKCOMES/MCC) and UK Summer Schools and DL_Software training. *Complete, DL_Software training workshops completed in November & December* • Collaborative Support. *On-going leading to 3 further minor releases and numerous community emails.*
	DL_FIELD	• Run and manage large-scale graphene-cellulose nanocomposite simulations. • Automatic introduction or removal of core-shell models. • Automation of setting up mixed organic/inorganic parameters with different mixing schemes.

UKCP	**CASTEP**	• meta-GGA Consistent pseudopotentials • Analytic first derivatives of meta-GGAs to enable geometry optimisations and molecular dynamics with this new functionality

UKCOMES	**DL_MESO**	• Improved form of cascaded LBE collision algorithm, with extension to additional three-dimensional lattice scheme (D3Q19) • Concave corner and edge boundary conditions

		• Release of version 2.7
	MPLB	• Body force implementation for shallow water equations in MPLB code • Implement 3D MPLB code and test using Taylor-Green vortex

HECBioSim	**Longbow v1.5.1**	• Bug fix - a number of parameters that are only used in specific scheduler or application plugins have been renamed to include the plugin name prefix. • Bug fix - executables expressed as absolute paths for supported plugins would cause a crash due to searching for a module with that key. • Bug fix - wrong error message was displayed when an executable didn't exist on HPC machine. • Bug fix - fix for crash when using NAMD SMP builds, the commandline parameters beginning with "+" would trigger the crash. • Bug fix - fixed misleading error messages about missing files and flags. • Bug fix - fixed problem where the newly added bash autocomplete did not allow filenames on disk to autocomplete. • Bug fix - fixed a problem when a large number of short jobs that trigger job subqueuing would cause a crash. • Bug fix - fixed user reported bug with strange looking error messages concealing a further absolute path bug. • Bug fix - Restored the ability to issue --maxtime on the commandline. • New feature - Added support for the slurm gres flag so users can do something like this "slurm-gres = gpu:1" in their host or job conf files. • New feature - support added for the upcoming release of python chemshell. • Bug fix - fix for problem where parameters in configuration files containing the "=" sign would cause the input file parser to misread them.

		• Bug fix - fix for problem with LAMMPS jobs where files provided with "include" or as part of other parameters would not be transferred, thanks to Anders Johansson for suggesting some ideas and solutions. • The structure of the Longbow API has been simplified, the source files no longer reside in a subdirectory called "core" within the installation directory. This has made importing much simpler and imports shorter. • Examples have been restructured and the how to run instructions updated. The actual run files remain the same, there are still incompatibilities with these and newer versions of MD codes but this will be addressed in the next version.
	Longbow v1.5.2	• Bug fix - OMP environment variable added to all schedulers to fix a specific set of user reported issues. • Bug fix - Further PBS and NAMD SMP issues relating to under subscription, users had to do a hacky way by dropping the corespernode parameter to under subscribe which resulted in errors from the scheduler. Now users wishing to do this should set mpiprocs in their job or host conf files to do this. • Bug fix - The memory parameter only worked with the PBS scheduler, this has now been extended to work in all schedulers. • Bug fix - The --maxtime parameter went missing from the --help output. • Doc fix - The documentation for the recovery mode was incorrect. • New feature - An update mode has been added so that users doing disconnectable sessions can simply run an update to get the current simulation status and download a snapshot of the data. • New feature - Move documentation to be under version control, using sphinx and readthedocs for auto documentation assembly. Documentation can then become part of the CI cycle and thus be enforced on code contribution.

		• Enhancement - users can now explicitly set the filenames of stderr and stdout from the scheduler script using the parameters "stdout = filename" and "stderr = filename" in their host of job conf files. • Enhancement - Users can now make use of existing job scripts, by providing the name of the script to the parameter "subfile" in their host or job conf files. This mode is mainly aimed at advanced users that understand the short falls of doing this and the problems that could occur. • Enhancement - Users can now set the naming scheme of the replicate directories. Instead of having to provide directories of the form rep1, rep2, ..., repx. Users can now set the name of the "rep" part by setting the "replicate-naming" parameter. So "replicate-naming = foo" would need directories named foo1, foo2, ..., foox. • Enhancement - Documentation for the examples have been cleaned up and added to the new sphinx docs. • Enhancement - Refactor the exception code in the top level API methods to remove duplication. • Removed support for Python versions 2.6, 3.2 and 3.3 due to these versions being old unsupported versions and various python packages such as pip/ci-tools withdrawing support. Longbow may still work for these versions but this is no longer guaranteed.
	Training Platform containers **V1.0.0**	A set of docker containers have been constructed that can be used to build powerful interactive Jupyter notebook training courses have been constructed. These are available via github and dockerhub.

UKCTRF	**HAMISH**	• Delivered a stable version for Cambridge and Newcastle researchers • Conversion of the code from f77 to f90 • Dynamic memory allocation

TRAINING AND OUTREACH

CCP5	CCP5 had a very busy and successful year when comes to **training both international and national.** In June we organised an international event CCP5/CCP_BioSim Molecular Simulation and Software Training School - Materials and Biomolecules organised at Universidad del Norte in Barranquilla, Colombia, 25-29 June 2018 was attended by 25 students and increasing the visibility of CCP5 in a part of the world where we did not have a presence. A similar Internationl event is planned for Q2 2019 at Universidad del Norte Antafagosta, Chile. A local three days training for CCP5 software was delivered in December 2018 at University of Manchester, 20 students participated and where induced to usage of DL_POLY, DL_FIELD, DL_MESO and ChemShell. At request of community Alin Elena has prepared and delivered at Queen Mary Univeristy two 2 days courses, **one Introduction to Modern Fortran and Introduction to MPI.** Both courses were attended by 30 students from UK universities. A two day course Introduction to QM/MM simulations with Chemshell was delivered at University of Bristol, 28 Feb- 1st of March coorganised with CCPBiosim. You Lu and Tom Keal hosted the first Py-ChemShell training workshop at Daresbury in January 2019 for six UCL students and PDRAs, using new training materials written for the redeveloped program. A follow up 3 days course is planned for Introduction to Modern Fortran in Q2-Q3 2019. **CCP5 Summer School 2018** was organised for the third and last year at University of Lancaster, in July 2018 for 11 days and was attended by 69 participants out of 92 applicants, from all over the world. We have introduced a two day programming lectubres (Python/Fortran) to help students be more efficient with the practicals. The school involved not only distinguished academic and industrial speakers (Jonathan Doye, Oxford, Michele Vendruscolo, Cambeidge, Therese Malavian, Institute Pasteur, Paris, Mike Allan, University of Bristol and Patrick Warren, Unilever) but also trainers and lecturers from other CoSeC consortia such as HEC-MCC, UKCOMES, CPUK and CCP5. **CCP5 Summer School 2019** has moved to Durham University, for the next three years. We had a number of 153 applications. 75 participants were selected this year. We have as returning lecturer Prof Mike Allan, one of the founders of the school. As invited speakers we have this year Daan Frenkel, Cambridge, Marialore Sulpizzi, Mainz, Mark Wilson, Durham, Fausto Martelli, IBM and Misbah Sarwar, Johnson Matthey. One needs to note the ascending trend in applications. Alin Elena delivered Introduction to HPC and benchmarking at the work experience week organised at Daresbury Laboratory for college students. Alin Elena has participated in two career fairs in Halton area, at Runcorn and Widnes Highschools. More than 500 students attended the events. Alin also has become a STEM Ambassador with activities planned at Manchester Science and Industry Museum in April 2019. Alin participated in Computer access day organised in Q4 2018 at Daresbury labs with more than 400 local children and parents participating.
CCP9	Organized/co-organized: • Widening participation workshop: Advanced Topics in Cs-corrected STEM and Spectroscopy: Theory meets Experiment, Daresbury Laboratory, 29 June 4 July 2018.

	• CCP9/CCP5 workshop: Simulation and modelling of nuclear materials, University of Bristol 4 – 5 June 2018. • Questaal hands-on course: Many-body response functions in the Questaal code, Daresbury Laboratory, 21 – 25 May 2018 • CCP9 Young Researchers Event and Community Meeting 2018, Park Inn Radisson, York 18-19 July 2018. • Physics by the Lake 2018, Cumberland Lodge, July 29 – August 10 2018. • Crystal school: MSSC2018 - Ab initio Modelling in Solid State Chemistry, Imperial College 17-21 September 2018. • The workshop "Forcefields: Status Challenges & Vision" Daresbury Laboratory, 28-29 January 2019. • Workshop on ab-initio Spin Modelling, Lausanne 26-28 November 2018 CCP9 furthermore provided funding: • Hermes Summer School 2018, Cumberland Lodge, 19 – 23 July 2018 • Hands-on course: ONETEP coding retreat, Cedar House, 10-14 September 2018 • 6th Computational Molecular Science Meeting, University of Warwick, 27 – 29 March 2019 • CASTEP User workshop, University of Birmingham, 18-19 March 2019 • 2nd joint CCP9-MCC-UKCP-EPCC workshop on ab-initio periodic codes, 21-24 January 2019 • New horizons in atomistic spin modelling, Bar Convent, York, 4 January 2019
CCPmag	Sponsored session at IoP conference – Magnetism 2018 (9-10 April 2018)
CCP-NC	As usual, CCP-NC people took part in the annual CASTEP Workshop in August. This consisted of a few talks introducing computational techniques for NMR and CCP-NC software (MagresView and Soprano) and support throughout the practicals.
CCPQ	Training activities provided by SLA/CoSeC for CCPQ members are generally in the form of specialized informal group meetings and one-to-one interactions (local and virtual). In this reporting period the 'scientific code' sessions have been concentrated in three areas: the Fortran 2003 code in the UKRMol+ suite and the necessary revisions needed for optimization; the incorporation of heavy-particle PFARM into RMAT_REACT and how to best use it, including (ongoing) training on the intricacies of the parallelism; the revisions to R-matrix theory and code needed to account for double continuum processes; use of GPU-BLAS in 'novel' technology versions of application codes; the applicaton of Feshbach resonance theory adapted to 'bound matter-antimatter states embedded in the continuum. In addition, SEG had regular discussions with M Lubasch (TNT code and repository manager) on how best to move the repository, and general discussions with the QUANTICS and RMT communities on the incorporation of the codes into ANVIL.
CCPPlasma / HECPlasma	Training in this period has focussed on issues around the GS2 migration to Bitbucket and git. We have given a number of one-to-one informal sessions on using new software, as well as providing support through our GS2 slack channel.

CCP PET-MR	Our main outreach activities during the reported period continued to be our regular (every 6 weeks) Software Framework meetings, where we discussed our development progress with our potential developers and users from PET-MR research community (KCL, Leeds, Manchester and other Universities' researchers) and representatives of major imaging scanner manufacturers, including Siemens and GE. CCP PET-MR has funding to support the exchange of researchers (staff and students) between institutions. Two exchange programs were supported in the reported period: between UCL and Physikalisch-Technische Bundesanstalt Berlin, Germany, and between UCL, Leeds and the Commonwealth Scientific and Industrial Research Organisation, Australia (the latter part-funded by CSIRO). These exchanges were supported by CoSeC staff when coding problems arose and to discuss design. Both exchanges led to substantial Pull Requests, currently under revision. The hackathons mentioned above also contained a large component of training. CCP PET-MR organised the one day PET-MRI School for students and early stage researchers at PSMR 2018, the 7th Conference on PET-MRI and SPECT-MRI in May 2018, La Biodola, Isola d'Elba, Italy (25 attendants) with a hands-on PET-MR software training session using SIRF. CoSeC staff helped in developing the training material and one joined the school for assistance on site. The school was very well received, with the hands-on sessions using Jupyter notebooks very much appreciated. CoSeC staff is also helping in preparing updated material for a similar course in April at PSMR 2019, Muenich, Germany. Due to feedback from last year, this year's course will have a larger fraction of time dedicated using our SIRF software.
CCPBioSim	• The ScotCHEM QM/MM Workshop, St Andrews was held on 14 June 2018, featuring ChemShell training for biomolecular simulations. 30 trainees attended. • CoSeC supported the CCPBioSim training workshop week at Bristol in April through provision of online workshop summaries and registration pages. • Simulations for Experimentalists and Industrialists, Diamond, 6-7 November 2018. Two lectures: 'Biomolecular Simulations' and 'QM/MM Calculations' were contributed to the CCP5 event. • Getting Started with Biomolecular Simulations, training workshop at the University of Leeds, 10-11 January 2019, 38 participants. • QM/MM modelling with ChemShell, University of Bristol, 28 Feb-1 Mar 2019, 19 participants.
UKCOMES	Three formal training events have taken place: a five-day CCP5/CCPBiosim Molecular Modelling School at Universidad del Norte, Barranquilla (25 participants) in June 2018, the CCP5 Summer School at Lancaster University in July 2018 and a DL_Software Training Workshop at the University of Manchester in December 2018. The events in Barranquilla and Lancaster included seminar talks on Dissipative Particle Dynamics provided by Michael Seaton, while all three included practical exercises using DL_MESO. Jianping Meng provided intensive one-on-one training to an MSc student, Yunlong Fei, at Sichuan University on the lattice Boltzmann modelling of shallow water flows and the usage of the MPLB code in August 2018.
MCC	• Leonardo Bernasconi contributed to the CCP5 Summer School on Molecular Simulation (Lancaster, July 2018)

	• Leonardo Bernasconi contributed to the MSSC 2018 CRYSTAL Summer School (Imperial College London, 2018) • Tom Keal gave an introduction to ChemShell at the MCC software training workshop held at the University of Lincoln on 3 September 2018 • Chin Yong presented an introduction to DL_FIELD at MCC Science Meeting (London, July 2018) • Chin Yong, Tom Keal and Barry Searle presented overviews of DL_POLY/DL_FIELD, ChemShell and CRYSTAL at the MCC Annual Conference (Lincoln, Sept 2018) • Chin Yong gave a DL_FIELD presentation and training at the CCP5/CCPBioSIm International MolSim School at Barranquilla, Colombia (25-29 June 2018), CCP5 Workshop for Experimentalist and Industrialists @ Diamond (5-7 November 2018), 2018 PRACE MolSim Winter School @ NCSA, Bulgaria (26-29 November), at DL_SOFTWARE Training @ Manchester (10-13 December 2018) • Ilian Todorov gave a DL_POLY presentation and training at Chin Yong gave a DL_FIELD presentation and training at the CCP5/CCPBioSIm International MolSim School at Barranquilla, Colombia (25-29 June 2018), CCP5 Workshop for Experimentalist and Industrialists @ Diamond (5-7 November 2018), 2018 PRACE MolSim Winter School @ NCSA, Bulgaria (26-29 November), at DL_SOFTWARE Training @ Manchester (10-13 December 2018) • Ilian Todorov gave outreach talks at Daresbury Laboratory (open public night May), First RSE-Netherlands Meetup (September 2018), UKCOMES International Workshop on Mesoscale Simulation and Modelling @ The Royal Society, London (5-6 November 2018), IOP Integrated Computational Materials Engineering Workshop (18 December 2018) and at Bilateral International Meeting organised by the Royal Society and the French Academy of Sciences (20-21 February 2019). • Barry Searle provided support for CRYSTAL training at the MCC-UKCP-EPCC workshop on periodic DFT codes at Daresbury in January. • Tom Keal provided Py-ChemShell training to six MCC members from UCL in January (with You Lu, CCP5).
HECBioSim	HECBioSim does not yet offer its own training programme with the training being delivered from CCPBioSim. However, HECBioSim has supported the development of the new CCPBioSim training platform. This platform consists of self-contained training courses that can be completed through a web interface (Jupyter) either individually or at a traditional training workshop or surgery. Due to the success of this training model with delivering developer led training that remains accessible and useable long into the future. Later in this working year, a new cloud version based on the Oracle cloud platform will be commissioned to deliver a wider array of training content via a single scalable resource. HECBioSim will contribute to managing this cloud based real estate, whilst CCPBioSim members will contribute training modules.
UKCTRF	Code_Saturne Training, 5 June 2018 Modern Fortran course, 6-10 August 2018 Cmake crash course, 20 March 2019

Software Outlook	The Online Mixed-Precision Training Course went live in August. There were problems with making the online TAU Training Course go live due to the large size of the Virtual Machine but this has now been resolved and the course added to the website. During this year, we have been working with many more CCPs and HEC consortia as part of our work packages. We have also made use of the Informal CoSeC Staff Meetings to gather information from different CCPs and HEC Consortia.

GLOSSARY

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

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

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

QM/MM	Coupled quantum mechanical and molecular modelling simulations
Quantics	A package based on the MCTDH algorithm for molecular quantum dynamics
Questaal	A suite of electronic structure programs. The codes can be used to model arbitrary materials, but they are mostly designed to answer condensed-matter theory questions about solid state (periodic) structures.
RAL	Rutherford Appleton Laboratory
R-Matrix Suite	A set of programs for electron (positron) -atom and -molecule scattering, (ultrafast) laser pulse interactions and related problems
RSE	Research Software Engineer
ScaleMP	Software that allows the creation of virtual shared memory systems
SCD	Scientific Computing Department
SESC	Software Engineering Support Centre
SIRF	Synergistic Image Reconstruction Framework developed by CCPPetMR
SISC	Journal on Scientific Computing
SKA	Square kilometre array project
SLA	Service Level Agreement
STFC	Science and Technology Facilities Council
TD-DFT	Time dependant density functional theory
TNT	A package coding Tensor Network Theory for coherent many-body nuclear dynamics
ToScA	Tomography for Scientific Advancement Symposium
UK-AMOR	UK Atomic, Molecular and Optical physics R-matrix Consortium
UKCP	The United Kingdom Carr-Parrinello Consortium
UK-COMES	UK Consortium on Mesoscale Engineering Sciences
UKCTRF	UK Consortium on Turbulent Reacting Flows
UKCRIC	UK Collaboration for Research on Infrastructure and Cities
UKTC	UK Turbulence Consortium
UKRI	UK Research and Innovation - the home of world class research and innovation in the UK