ARCHER CSE Service Quarterly Report

Quarter 3 2014

1. Executive Summary

This report covers the period: 1 July 2014 to 30 September 2014 inclusive.

- Centralised CSE Team:
  - The CSE team resolved 413 queries during this reporting period.
  - The number of In-Depth queries resolved fell from 80 in Q2 to 46 in Q3 (97 were resolved in Q1 2014). The lower number of queries indicates that users are more familiar with the system and that there are fewer requests to install new software.
  - The median resolution time for In-Depth queries is 4 weeks.
  - The median completion time for Technical Assessments is 4 days.
- Summary of feedback
  - Feedback on query handling uniformly rated the service as "Excellent".
- Training:
  - Provided 22 days (631 student-days) of face-to-face training in the quarter, at 7 different locations.
  - Provided 1.5 days of virtual tutorials as interactive webinars with more than 80 attendees in total, an increase over the previous quarter's attendance of 60.
  - GPU course in Sheffield used as "train the trainers" event: ARCHER material was delivered by local staff but additional tutorial support was provided by EPCC.
  - Joint ARCHER/DiRAC training course on manycore / Xeon Phi programming agreed in principle, and will form part of proposed 2015 training plan.
  - Survey for measuring longer-term impact of training approved by ARCHER Training Panel. This will be circulated to course attendees on a regular basis; first set of attendees have been contacted. See http://archer.ac.uk/training/feedback/follow-up-survey.php
  - Meeting of ARCHER Training Panel arranged for 15 October to discuss proposed training plan for 2015.
- eCSE:
  - Of 14 projects accepted for the first call, 13 have started with all associated contracts signed and costs agreed. The one remaining project is undergoing a change of staffing.
  - Of 9 projects accepted for the second call, 8 have started with all associated costs agreed. Contracts are in the process of being agreed and signed. The one remaining project is undergoing a change of staffing.
  - The third eCSE call opened on 5 August 2014 and closed on 16 September, receiving 16 proposals.
  - Templates for interim eCSE reports have been agreed.
  - Outline of final eCSE reports has been agreed along with outline of reviewing process for completed projects.

2. Impact Summary

- Outreach Activities:
  - 26 September 2014: Meet the Experts, Our Dynamic Earth, Edinburgh (http://www.explorathon.co.uk/edinburgh/meet-the-experts)
  - 14 September 2014: Bang Goes the Borders, Melrose (http://www.bgtb.org/)
  - 6-11 September 2014: British Science Festival, Birmingham (https://www.epcc.ed.ac.uk/blog/2014/09/10/epcc-british-science-festival-2014)
  - 10 July 2014: Sutton Trust, Medical School, University of Edinburgh (http://www.ph.ed.ac.uk/news/sutton-trust-04-08-14)
- Papers from Centralised CSE Team:
  - **Linear instability, nonlinear instability and ligament dynamics in three-dimensional laminar two-layer liquid-liquid flows,** L. Ó Náraigh (Dublin), P. Valluri (Engineering Edinburgh)**,** D. Scott (EPCC Edinburgh), I. Bethune (EPCC Edinburgh) and P. D. M. Spelt (Lyon), *Journal of Fluid Mechanics*, 750, p464-506
  - **targetDP: an Abstraction of Lattice Based Parallelism with Portable Performance**, Alan Gray and Kevin Stratford, HPCC 2014 conference, Aug 2014, proceedings at arxiv.org/abs/1405.6162
- Conference Presentations from Centralised CSE Team:
  - **Route towards droplet formation in laminar separated liquid/liquid flows: analysis and large-scale DNS using TPLS**, The Geoff Hewitt Celebration Conference on Multiphase Flows, Imperial College London (July 2014)
  - **Ultra-high resolution direct numerical simulations of stratified flows: From waves to droplet pinch-off**, First Thermapower Workshop, Shanghai (Aug 2014)
- Meetings Attended by Centralised CSE Team:
  - UK Turbulence Consortium Annual Review (22-23 September 2014). Consortium Contact met users and discussed how CSE service can help them and opportunities for code improvement.
  - HPC-SIG (30 September 2014, Imperial College, London). Discussed links between regional/institutional HPC and national HPC. Continue to build links with UK HPC community.
  - ARCHER Upgrade Consultation Workshop (10 July 2014, London). Provided technical input to discussion of Phase 2 upgrade options.
- Presentations by Centralised CSE team:
  - Lecture on "HPC Architectures" at the EPSRC-funded "HPC Autumn Academy" (15-26 September 2014, Cambridge). This school is aimed at EPSRC-funded PhD students and early-stage researchers in computational science.

3. Continual Service Improvement

- Centralised team:
  - Reduction in volume of In-Depth technical queries has allowed us to put more effort into proactive technical activities. For example, producing documentation on best practice in parallel IO, on monitoring power consumption by user jobs, and on using Python in HPC.
  - Plans to produce short online "how to" screencast videos on using particular tools: debuggers, profilers, etc. to complement the online written documentation.
- Consortium Contacts:
  - Start developing links with major users from Consortia as well as with PI's.
  - Monitor and report on Consortium usage profiles to PIs.
- Performance monitoring:
  - Analysis of time to completion of Technical Assessments now included in this report. Should help inform metric development in future.
- Website development:
  - Knowledgebase of compilation instructions for scientific software packages now available on website. Will continue to expand and improve this information. This aids ARCHER users, staff and the worldwide HPC community.
  - CSE staff profiles now available on the website. Plan to add photographs and publicise to users. Aim to give "faces" to the ARCHER service.
- Technical Forum:
  - Presentations in TechForum Webinar series from first batch of eCSE projects. Showcase the advances made possible through eCSE funding.
  - Initial set of webinar recordings now available on website. Remainder are being processed.
  - Mailing list renamed to "hpc-techforum" to encourage sharing of expertise from all HPC users, ARCHER and otherwise.
- New Scientific Python training developed due to increased demand
  - Extra day on Python programming added to July's Software Carpentry course.
  - August virtual tutorial on Python attracted in excess of 45 attendees.
- Online material
  - Material from all ARCHER courses now available online after each course run.
  - Recordings of virtual tutorials are now being posted on youtube channel "ARCHER High Performance Computing Service."
  - Designed a feedback form tailored for online courses which we will use after all virtual tutorials. It will also be available for people to fill in after they have watched any of the online videos.
- eCSE:
  - Based on feedback from the previous eCSE panel meeting, review functionality being improved in the SAFE for reading the associated proposal and review documents.
- Raising profile of science enabled by ARCHER
  - ARCHER Image Competition opened; closing at end of October. Images will be used to promote the scientific impact of ARCHER.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: July 2014, August 2014 and September 2014.

The metrics were specified by EPSRC in Schedule 2.2 of the CSE Service Contract.

CSE Query Metrics

- **QE1:** The percentage of all queries notified to the Contractor by the Help Desk in a Quarter that the Contractor responds to, and agrees a work plan with, the relevant End User within 3 working hours of receiving the notification from the Help Desk. *Service Threshold: 97%; Operating Service Level: 98%.*
- **QE2:** The percentage of all queries notified by the Help Desk to the Contractor that have been satisfactorily resolved or otherwise completed by the Contractor within a 4-month period from the date it was first notified to the Contractor. *Service Threshold: 80%; Operating Service Level: 90%.*
- **TA1:** The percentage of all technical assessments of software proposals provided to the Contractor by the Help Desk in any Service Period that are successfully completed by the Contractor within 10 days of the technical assessment being provided to the Contractor by the Help Desk. *Service Threshold: 85%; Operating Service Level: 90%.*
- **FB1:** The percentage of End User satisfaction surveys for CSE queries carried out in accordance with the Performance Monitoring System by the Contractor showing the level of End User satisfaction to be "satisfactory", "good" or "excellent". *Service Threshold: 30%; Operating Service Level: 50%.*

Period	Jul-14		Aug-14		Sep-14		Q3 2014	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
QE1	100%	-2	100%	-2	100%	-2	100%	-6
QE2	100%	-2	100%	-2	100%	-2	100%	-6
TA1	100%	-1	92%	0	100%	-1	96%	-2
FB1	100%	-2	100%	-2	100%	-2	100%	-6
Total		-7		-6		-7		-20

Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level

Training Metrics

- **FB2:** The percentage of all training satisfaction carried out in accordance with the Performance Monitoring System by the Contractor) in each Quarter that are rated "good", "very good" or "excellent". *Service Threshold: 70%; Operating Service Level: 80%.*

Period	Jul-14		Aug-14		Sep-14		Q3 2014	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
FB2	100%	-1	100%	-1	100%	-1	99%	-3
Total		-1		-1		-1		-3

Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level

5. CSE Queries

Queries Resolved in Reporting Period

Metric Descriptions

In-Depth	All technical queries passed to ARCHER CSE team
Course Registration	Requests for registration on ARCHER training courses or enquiries about registration
Technical Assessment: <Category>	Request for Technical Assessments of applications for ARCHER time
eCSE Application	Queries relating to eCSE applications

A total of 413 queries were resolved by the CSE service in the reporting period.

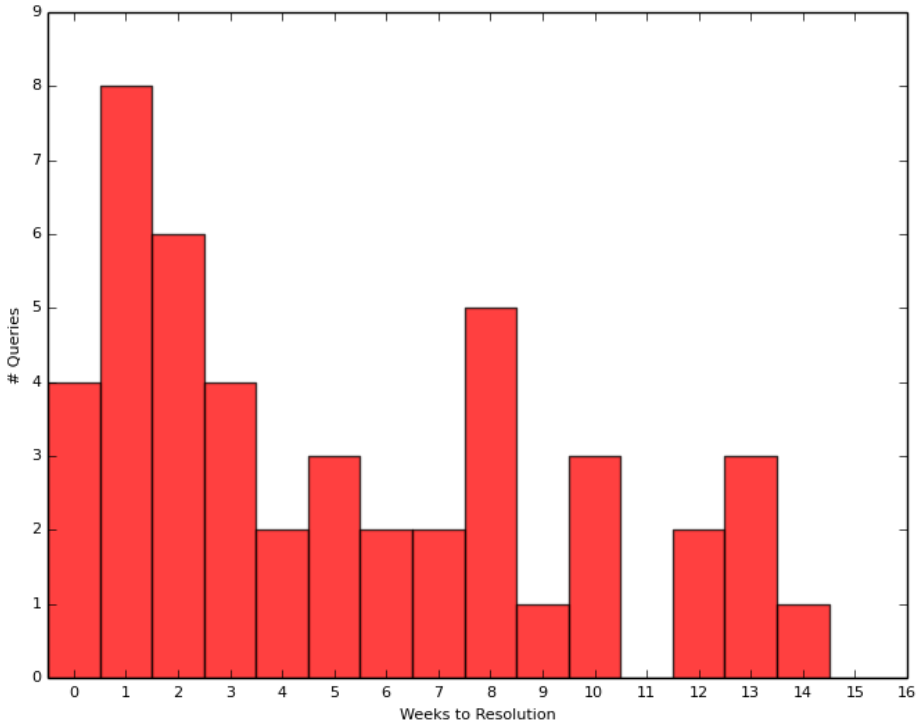
Metric	Jul-14	Aug-14	Sep-14	Total	% Total
In-Depth	20	12	14	46	11.1%
Course Registration	223	26	38	287	69.5%
Technical Assessment: Grant	10	4	9	23	5.6%
Technical Assessment: RAP	0	6	14	20	4.8%
Technical Assessment: Instant	5	2	3	10	2.4%
Technical Assessment: HEC	1	0	7	8	1.9%
eCSE Application	6	3	10	19	4.6%

All of the feedback left by users on queries was rated “Excellent”. 9 query feedback responses were received on In-depth queries in the reporting period. This represents a 20% return rate for feedback forms.

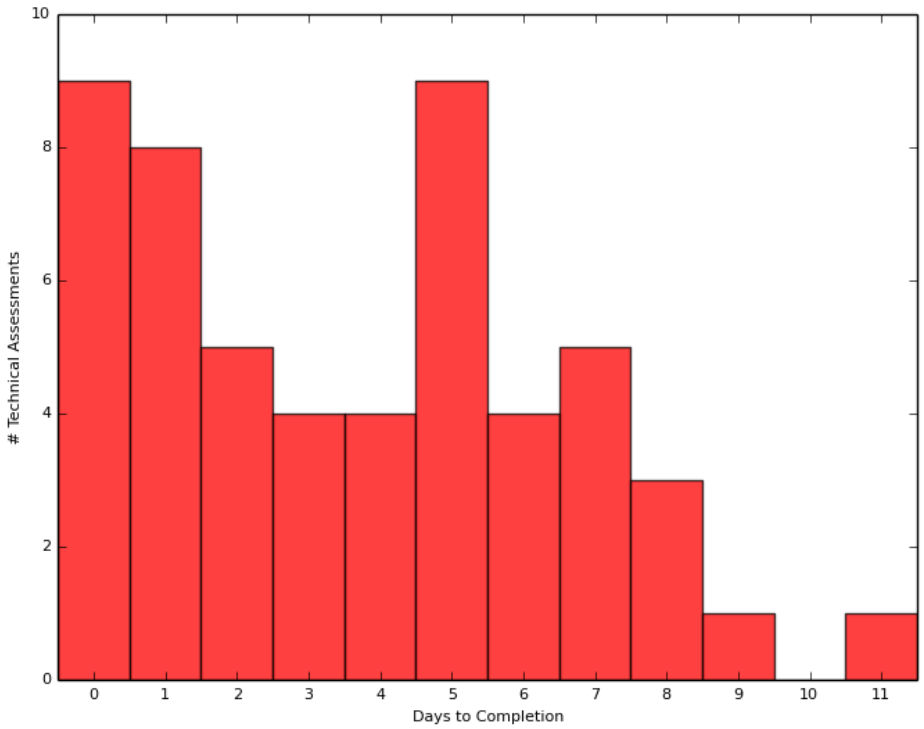
Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	31	67.4%
Compilers and system software	4	8.7%
User Programs	3	6.5%
Performance and scaling	2	4.3%
Batch system and queues	2	2.5%
Other	2	4.3%
User behaviour	1	2.2%
Porting	1	2.2%

A histogram of the time to resolution for In Depth queries (see below) reveals that the median resolution time is 4 weeks.



A histogram of the time to completion for Technical Assessments (see below) reveals that the median completion time is 4 days.



6. Training

The CSE Service has provided a total of 22 days (631 student-days) of face-to-face training across seven different locations in the reporting period, plus 1.5 days of interactive web-based training. The table below summarises the training delivered in Q3 2014.

Month	Dates	Course	Location	Days	Attendees
Jul 2014	30 Jun – 4 Jul	ARCHER Summer School	EPCC	5	31
	1	GPU Programming with CUDA	Sheffield	1	30
	9	Virtual Tutorial: Make and Compilation issues	Online	0.5	
	21-23	Software Carpentry and Scientific Python	Cranfield	3	37
Aug 2014	13	Virtual Tutorial: Python for High Performance Computing	Online	0.5	
	18-19	Introduction to F95	Culham	2	12
	20-21	Introduction to OpenMP and MPI	Culham	2	13
	27-28	NSCCS/ARCHER CP2K Workshop 2014	London	2	41
Sep 2014	1-2	GPU Programming	Edinburgh	2	45
	2-3	Efficient Parallel IO on ARCHER	Daresbury	2	12
	3	Introduction to ARCHER	Edinburgh	1	21
	3	Virtual Tutorial: Tools for Building and Submitting an eCSE Proposal	Online	0.5	
	16-17	Software Carpentry	London	2	34

On the feedback forms, attendees rated the course on a scale of 1-5 ("Very bad", "Bad", "Good", "Very good" and "Excellent". The average feedback using this metric was 4.3, i.e. better than "Very Good". Users provided 192 feedback forms on the CSE courses.

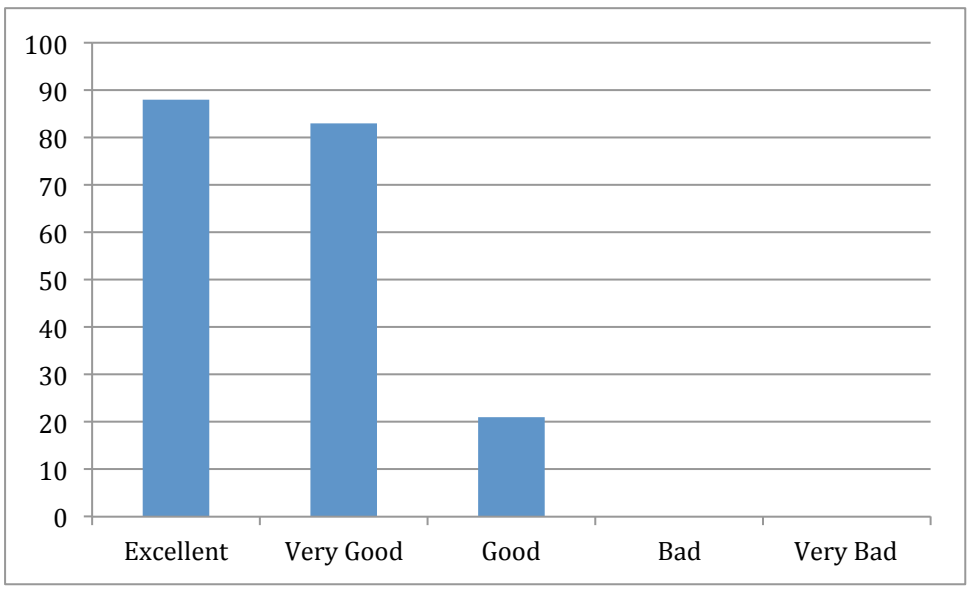


Figure 1: Breakdown of feedback responses from training course surveys for Q3 2014.

13.5 days of training are currently planned for the following quarter. Details are provided in the table below. All face-to-face courses have been opened for registration except for "Shared-Memory Programming with OpenMP" in Durham where we are in the process of finalising local arrangements.

Month	Dates	Course	Location	Days
Oct 2014	8	Virtual Tutorial: Parallel IO and the ARCHER Filesystem	Online	0.5
	21-22	Hands-on Introduction to HPC	London	2
	23-24	Message-Passing Programming with MPI	London	2
Nov 2014	12	Virtual Tutorial: Software Revision Control	Online	0.5
Dec 2014	3-4	Shared-Memory Programming with OpenMP	Durham	2
	3-4	Software Carpentry Workshop	Edinburgh	2
	10	Virtual Tutorial: Intro to GPU programming	Online	0.5
	16-17	Hands-on Introduction to HPC	Southampton	2
	16-17	Single Node Performance Optimisation	Cambridge	2

7. Embedded CSE (eCSE)

eCSE Call 1

- 13 out of 14 projects agreed/contract signed and started.
- Costs agreed for 13 out of 14 projects
- For the one exception, Panel agreed that PI and eCSE team were to identify alternative staffing.

eCSE ID	PI	Title	PMs	Status
eCSE01-001	Michail Stamatakis <m.stamatakis@ucl.ac.uk>	Zacros Software Package Development: Pushing the Frontiers of Kinetic Monte Carlo Simulation in Catalysis	12	Started 01/09/14
eCSE01-002	Dr Alan Gray < a.gray@ed.ac.uk>	Introducing Thread and Instruction Level Parallelism into Ludwig	12	Started 01/09/14
eCSE01-003	Dr Benedict Rogers <benedict.rogers@manchester.ac.uk> (Manchester)	Developing highly scalable 3-D incompressible SPH	12	Started 01/09/14
eCSE01-004	Chris-Kriton Skylaris <c.skylaris@soton.ac.uk> (Southampton)	A pinch of salt in ONETEP's solvent model	3	Started 01/06/14
eCSE01-005	Mark van Schilfgaarde <mark.van_schilfgaarde@kcl.ac.uk>(KCL)	QuasiParticle Self-Consistent GW calculations of many-atom systems	6	Started 01/08/14
eCSE01-008	Dr. Prashant Valluri <Prashant.Valluri@ed.ac.uk>(Edinburgh)	TPLS: Optimised Parallel I/O and Visualisation	8	Started 01/04/14
eCSE01-009	Dr Gerard Gorman<g.gorman@imperial.ac.uk>	Scalable and interoperable I/O for Fluidity	6	Started 01/07/14
eCSE01-010	Dr Miguel O. Bernabeu<miguel.bernabeu@ucl.ac.uk> (UCL)	Adding a resolved deformable particle model to a highly-parallel blood flow solver for sparse vascular networks	12	Started 01/09/14
eCSE01-013	Jimena Gorfinkiel <Jimena.Gorfinkiel@open.ac.uk>(Open)	Efficient computation of two-electron integrals in a mixed Gaussian/B-spline basis.	12	Started 16/06/14
eCSE01-015	Professor Michael J Fagan <m.j.fagan@hull.ac.uk>(Hull)	Large scale voxel based modelling	15	Started 01/04/14
eCSE01-016	Dr Massimo Bollasina<massimo.bollasina@ed.ac.uk>	Porting and enabling use of the Community Earth System Model on ARCHER	4	Started 01/04/14
eCSE01-017	Dr Matt Probert <matt.probert@york.ac.uk> (York)	Hybrid OpenMP and MPI within the CASTEP code	12	Started 01/07/14
eCSE01-018	Scott M. Woodley <Scott.Woodley@ucl.ac.uk> (UCL)	Tuning FHI-Aims for complex simulations on CRAY HPC platforms	12	Started 01/06/14
eCSE01-019	lian Todorov <Ilian.todorov@stfc.ac.uk> (STFC)	DL_POLY_4: Multiple Time Stepping Development Support	6	Awaiting staffing change

eCSE Call 2

- 17 Proposals received through SAFE (1 subsequently withdrawn due to staffing issues in the project)
    - Withdrawn proposal planned for resubmission once appropriate local staff can be identified by PI.
- 9 proposals were successful
- 8 out of 9 projects agreed/contract signed and started
- One exception due to member of proposed staff taking up new post; PI in process of recruiting new employee

eCSE ID	PI	Title	PMs	Status
eCSE02-2	Prof Jason M Reese, Edinburgh	Multi-Scale Engineering Flow Simulation: Hybrid MPI/OpenMP Optimization on ARCHER	12	Started 20/09/14
eCSE02-3	Dr. Patrick E. Farrell, Oxford	Scalable automated parallel PDE-constrained optimisation for dolfin-adjoint	8	Started 01/09/14
eCSE02-6	Prof Hugo van der Hart, QUB	Performance enhancement of RMT codes in preparation for the treatment of circular polarization	9	Started 01/10/14
eCSE02-8	Dr David Dickinson, York	Optimising Field Solves in GS2: Improved load balancing and non-blocking communications for maximal efficiency at high #core	7	Started 01/09/14
eCSE02-9	Dr Matt Probert, York	Optimising van der Waals simulations with the CASTEP code	7	Started 01/08/14
eCSE02-11	Dr Nicolae Panoiu, UCL	Fast and Massively Distributed Electromagnetic Solver for Advanced HPC Studies of 3D Photonic Nanostructures	12	Awaiting recruitment
eCSE02-13	Prof Spencer Sherwin, Imperial College	Communication and I/O masking for increasing the performance of Nektar++	12	Started 01/10/14
eCSE02-15	Dr Nicholas Hine, Cambridge	Calculating Excited States of Extended Systems in LR-TDDFT	6	Started 01/10/14
eCSE02-17	Dr James Harle, Proudman Oceanographic Laboratory	NEMO Regional Configuration Toolbox	9	Started 01/10/14

eCSE Call 3

- 16 proposals received
- 162 person months requested in total

eCSE ID	PI	Title	PMs	Status
eCSE03-1	Prof. Tony Arber <t.d.arber@warwick.ac.uk> (University of Warwick)	Optimisation of the EPOCH laser-plasma simulation code	12	Submitted
eCSE03-2	Dr. Michele Sergio Campobasso <m.s.campobasso@lancaster.ac.uk> (Lancaster University)	Reducing the run-time and improving the ease-of-use and portability of the COSA 3D harmonic balance Navier-Stokes solver for open rotor unsteady aerodynamics	7	Submitted
eCSE03-3	Dr David J Huggins <djh210@cam.ac.uk> (University of Cambridge)	Algorithmic Enhancements to the Solvaware Package for the Analysis of Hydration	6	Submitted
eCSE03-4	Prof George Barakos <g.barakos@liverpool.ac.uk> (University of Liverpool)	Discrete velocity methods for the Helicopter Multi-Block CFD solver	12	Submitted
eCSE03-5	David R Bowler <david.bowler@ucl.ac.uk> (University College London)	The first general release of the linear-scaling DFT code Conquest with focus on the emerging field of biological simulations	12	Submitted
eCSE03-6	Dr Ozgur Yazaydin <ozgur.yazaydin@ucl.ac.uk> (University College London)	QM/MM Interfacing and Parallelisation of RASPA Molecular Simulation Package	12	Submitted
eCSE03-7	Dr Matthew Piggott <m.d.piggott@imperial.ac.uk> (Imperial College London)	Delivering a step-change in performance and functionality to the Fluidity shallow water solver through code generation	12	Submitted
eCSE03-8	James R. Maddison <j.r.maddison@ed.ac.uk> (University of Edinburgh)	Parallel supermeshing for multimesh modelling	8	Submitted
eCSE03-9	Dr Dan Jones <dannes@bas.ac.uk> (British Antarctic Survey)	Providing the ARCHER community with adjoint modelling tools for high-performance oceanographic and cryospheric computation	9	Submitted
eCSE03-10	Dr Garth Wells <gnw20@cam.ac.uk> (University of Cambridge)	High performance multi-physics simulations with FEniCS/DOLFIN	6	Submitted
eCSE03-11	Dr Matthew B Watkins <matthew.watkins@ucl.ac.uk> (UCL)	Local excitement in CP2K	12	Submitted
eCSE03-12	Xuerui Mao <xuerui.mao@durham.ac.uk> (Durham University)	Full parallelism of calculations of optimal flow control	12	Submitted
eCSE03-	Dr Rupert Nash	Grids in grids: hierarchical grid	12	Submitted

13	<rupert.nash@ed.ac.uk> (EPCC)	generation and decomposition for a massively parallel blood flow simulator		
eCSE03-14	Dr Irene Moulitsas <i.moulitsas@cranfield.ac.uk> (Cranfield University)	PGAS Fortran Coarray parallelisation strategies for CFD applications	12	Submitted
eCSE03-15	Dr Justin R Finn <J.Finn@liverpool.ac.uk> (University of Liverpool)	CFD2LCS: A general purpose library for integrated computation of Lagrangian coherent structures during massively parallel hydrodynamic simulations.	12	Submitted
eCSE03-16	Prof Jonathan W Essex <j.w.essex@soton.ac.uk> (University of Southampton)	Implementation of Dual Resolution Simulation Methodology in LAMMPS	6	Submitted

Future eCSE Calls

eCSE calls are run to a regular schedule. The upcoming calls are:

- eCSE Call 4: Opens 25 Nov 2014, Closes 13 Jan 2015