



ARCHER CSE Service Quarterly Report

Quarter 2 2014



1. Executive Summary

This report covers the period: 1 April 2014 to 30 June 2014. Results from the eCSE 2 panel meeting are also included even though it fell just outside this period as the information from the panel meeting is more relevant here than in the Q3 2014 report.

- Centralised CSE Team:
 - 342 queries were resolved by the CSE team during this reporting period, which is almost double the numbers in Q1 2014.
 - The large increase is due to a change that routes all training registrations through the ARCHER helpdesk. If Course Registrations are discounted then 149 queries were resolved.
 - The number of In-Depth queries resolved fell from 97 in Q1 to 80 in Q2. The lower number of queries reflects the fact that users are bedded-in to the service.
 - The median resolution time for In-Depth queries is 3-4 weeks.
 - Additional notifications added in SAFE for handlers of Technical Assessments and In Depth queries to improve responsiveness to users.
 - Using the SAFE to analyse resolution times for different classes of query (e.g. In-Depth, Technical Assessments).
 - Preliminary findings included in this report.
 - Each funded eCSE project has been assigned a named contact in the centralised CSE team to provide guidance and support throughout the project.
 - Provided technical input at ARCHER RAP, SAC and SMB meetings.
 - Attended EPSRC HEC Consortia heads meeting and provided update on CSE service activities.
- Summary of feedback
 - Feedback on query handling uniformly rated the service as “Excellent”.
 - Many responses commented on the rapid resolution of queries.
- Training:
 - Provided 20 days (526 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 60 attendees in total.
 - Organised joint CP2K course with NSCCS for Q3 2014.
 - In contact with DiRAC training manager about organizing joint training.
 - With PRACE funding, provided 15 travel bursaries of up to £400 each for researchers to attend the ARCHER Summer School at EPCC. More than 45 applications for bursaries were received.
 - Proposal for mechanisms for measuring impact sent to ARCHER Training Panel and discussed at a Panel meeting with invited EPSRC representative
- eCSE:
 - Preparations began for the 14 projects accepted from the first eCSE call.
 - Contract discussions took place with all other parties involved in eCSEs with most contracts signed or close to being signed.
 - The second eCSE call was opened on 1 April 2014 and closed on 13 May 2014 receiving 17 proposals (1 since withdrawn).
 - The second eCSE panel meeting took place on 8 July 2014; 9 proposals were successful.
 - New SAFE functionality was developed and deployed to enable proposals to be received and reviewed on-line.
- Technical Forum:
 - Speakers from EPCC, STFC and Cray presented webinars to a total of more than 50 attendees during the quarter.

2. Impact Summary

- Article on The Conversation website by Alan Simpson and Andy Turner
 - *So supercomputers are mega-powerful, but what can they actually do?*
 - <http://theconversation.com/so-supercomputers-are-mega-powerful-but-what-can-they-actually-do-24987>.
- Contributed a chapter describing ARCHER to latest edition of *Contemporary High Performance Computing* book
 - Edited by Jeffrey Vetter of Oak Ridge National Laboratory, USA.
 - Publication date to be confirmed.
- Outreach activities
 - Edinburgh International Science Festival, 5-9 April 2014. Interactive exhibit in National Museum of Scotland: *What makes supercomputers super?*
 - St. Peter's Primary School, Edinburgh, 14 May 2014. Supercomputer-based activities with 80 children from different age groups.
 - Tweedbank Nursery, Tweedbank Community Centre, 10 June 2014. Interactive session on supercomputers with around 30 children.
- ARCHER presented at a number of meetings
 - NA-HPC Meeting, 16-17 April 2014 (<http://www.mims.manchester.ac.uk/na-hpc/>).
 - G8 Project Meeting, Princeton.
 - ScotCHEM Computational Chemistry Symposium, 6 June 2014.
 - Women in HPC meeting, Thursday 24th April 2014.
- HPC-SIG
 - Provided update on ARCHER CSE Activities at HPC-SIG Meeting, QMU London, 15 May 2014.
 - Interest in putting together database of HPC libraries aimed at users.
 - Number of requests for CSE training at HPC-SIG sites.
 - Raised awareness of software porting and installation expertise available to all HPC providers in UK.
- International Supercomputing 2014 (ISC'14)
 - ARCHER promoted at EPCC booth on exhibition floor, and by EPCC staff attending.
- Women in HPC meeting
 - 33 attendees from across the UK.
 - Four invited talks talking on a range of subjects from ARCHER, to using HPC for simulating turbulent flows, and a varied career in the world of HPC.
 - Discussion in the Q&A session highlighted the importance of reaching out to women early in the careers, including tailoring the advertising of undergraduate and masters programmes to attract women. The discussion also highlighted the importance of mentoring and role models for retention of women in the HPC community and career progression.

3. Continual Service Improvement

- Performance monitoring
 - Further SAFE analysis planned to inform future service improvement and possible metric rationalisation for current and future services.
- Course Registration through SAFE
 - Allow us to manage the course lifecycle more efficiently
 - Enable collection of data on how training impacts a user's ARCHER usage profile.
- Move Technical Assessment process into SAFE
 - Convenience of completing online for users and reviewers.
 - Tailor questions to application type.
 - Closer integration in SAFE allows for more efficient process and improves service for users.
- Website development
 - Put CSE staff profiles online – visibility of CSE team to user community
 - Develop online knowledgebase of compilation instructions for centrally-installed scientific simulation packages.
 - Add in historical Technical Forum recordings for people who could not attend.
- Technical Forum
 - Rename Technical Forum mailing list to encourage expertise sharing between ARCHER, DiRAC and other HPC experts.
 - Publish TechForum webinar recordings online.
 - Encourage eCSE technical staff to give webinar presentations.
- Training
 - Ask users to complete online bash shell competency before attending introductory courses to maximise engagement with practical material.
 - Proposed survey form to be updated and circulated for final approval.
 - Plan to issue survey in Q3.
- eCSE
 - Further refinement to be completed based on feedback from the eCSE panel.
 - Plans to refine submission forms to include key success metrics to allow clear criteria for final assessment of projects.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: April 2014, May 2014 and June 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	Apr-14		May-14		Jun-14		Q2 2014	
	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	83%	1	96%	-1	100%	-1	96%	-1
FB1	100%	-2	100%	-2	100%	-2	100%	-6
Total		-5		-7		-7		-19

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

Single Technical Assessments (TA) took longer than 10 days to return to the applicant in each of April and May. This led to the failure in metric TA1 in April 2014 (due to the low number of requested TAs). Changes in the SAFE now provide automated reminders to the staff completing the TAs; this has aided the improvement in performance in June 2014. We plan to put additional processes in place (see Forward Look section above) to improve performance with TA completion.

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	Apr-14		May-14		Jun-14		Q1 2014	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
FB2	97%	-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

Single bad response in April as student did not have sufficient basic computing experience to engage with the practical exercises. Plan to add online crib sheet and tie in to existing Software Carpentry material for attendees prior to attending courses.

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 313 queries were resolved by the CSE service in the reporting period.

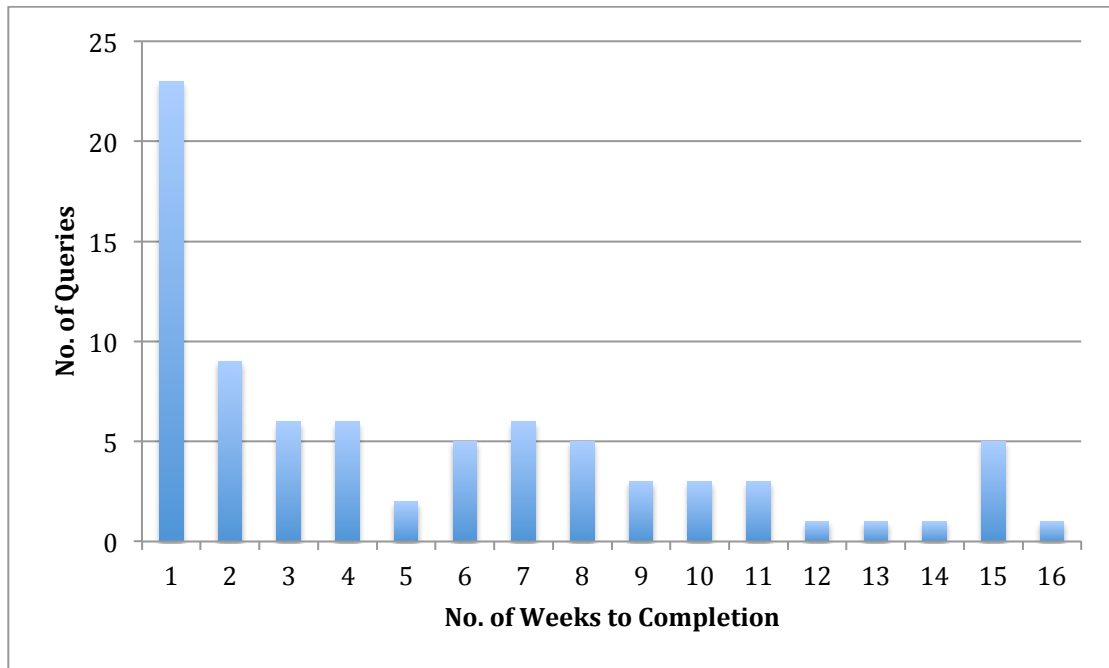
Metric	Apr 2014	May 2014	Jun 2014	Total	% Total
In-depth	33	23	24	80	23.4%
Course Registration	32	155	6	193	56.4%
Technical Assessment: Grant	0	13	7	20	5.8%
Technical Assessment: RAP	2	15	0	17	5.0%
Technical Assessment: Instant	0	3	5	8	2.3%
Technical Assessment: HEC	1	0	1	2	0.6%
Technical Assessment: Other	4	0	0	4	1.2%
eCSE Application	15	3	0	18	5.3%

All of the feedback left by users on queries was rated "Excellent". 14 query feedback responses were received on In-depth queries in the reporting period. This represents a 17.5% return rate for feedback forms.

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	59	73.8%
User programs	8	10.0%
Compilers and system software	4	5.0%
Performance and scaling	3	3.8%
Batch system and queues	2	2.5%
Other	2	2.5%
User behaviour	1	1.2%
Disk, tapes, resources	1	1.2%

A histogram of the time to resolution for In Depth queries (see below) reveals that the median resolution time is between 3 and 4 weeks.



6. Training

The CSE Service provided a total of 20 days (526 student-days) of face-to-face training across 7 different locations in the reporting period, plus 1.5 days of interactive web-based training. The table below summarises the training delivered in Q2 2014.

Month	Dates	Course	Location	Days	Attendees
Apr 2014	9-11	Intro to HPC and ARCHER	York	3	65
	16	Virtual Tutorial: PBS Job Submission	Online	0.5	
	23-25	Parallel Materials Modeling Packages	London	3	31
May 2014	23-24	Intro to HPC and ARCHER	EPCC	2	23
	29-1	Tools for Large-Scale Parallel Debugging and Profiling	EPCC	3	14
	6-8	Advanced OpenMP	Oxford	3	16
	12-13	Introduction to F95	Daresbury	2	23
	14	Virtual Tutorial: ARCHER Filesystems	Online	0.5	
Jun 2014	29-30	Statistical Analysis for Post-Genomic Data: Parallel Computing with R	Swansea	2	14
	4-5	Programming the Xeon Phi	Bristol	2	18
	11	Virtual Tutorial: Parallel Programming Models	Online	0.5	

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 4.2, i.e. better than “Very Good”. Users provided 80 feedback forms on the CSE courses.

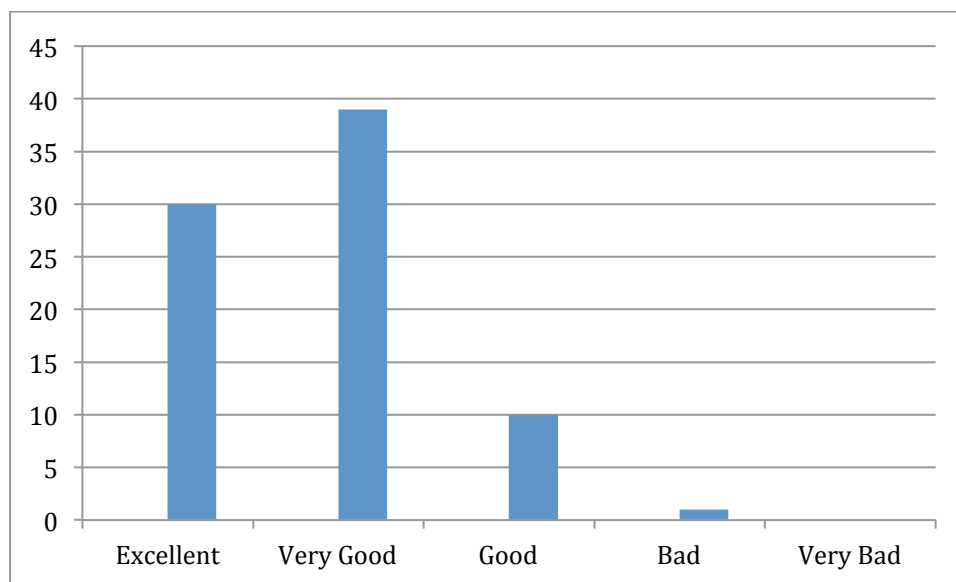


Figure 1: Breakdown of feedback responses from training course surveys for Q1 2014.

21.5 days of training are currently planned for the following quarter. Details are provided in the table below. All courses have been opened for registration.

Month	Dates	Course	Location	Days
Jul 2014	30 Jun - 4	ARCHER Summer School	EPCC	5
	1	GPU Programming with CUDA	Sheffield	1
	9	Virtual Tutorial: Make and Compilation issues	Online	0.5
	21-23	Software Carpentry and Scientific Python	Cranfield	3
Aug 2014	13	Virtual Tutorial: Title TBC	Online	0.5
	18-19	Introduction to F95	Culham	2
	20-21	Introduction to OpenMP and MPI	Culham	2
	27-28	NSCCS/ARCHER CP2K Workshop 2014	London	2
Sep 2014	1-2	GPU Programming	Edinburgh	2
	2-3	Efficient Parallel IO on ARCHER	Daresbury	2
	3	Introduction to ARCHER	Edinburgh	1
	10	Virtual Tutorial: Title TBC	Online	0.5

7. Embedded CSE (eCSE)

eCSE Call 1

- 8 out of 14 projects agreed/contract signed and started.
- 5 projects due to start by September
- Costs agreed for 13 out of 14 projects
- 1 exception due to cost. PI and eCSE team to identify alternative staffing, as agreed by the panel.

eCSE Call 2

- 17 Proposals received through SAFE (1 since withdrawn)
- Panel meeting on 8 July 2014
- 9 proposals were successful

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

Future eCSE Calls

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

- eCSE Call 3: Opens 5 Aug 2014, Closes 16 Sep 2014
- eCSE Call 4: Opens 25 Nov 2014, Closes 13 Jan 2015