ARCHER and ARCHER2 CSE Quarterly Report

April – June 2020

EPCC

The University of Edinburgh

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Document Information and Version History

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Reviewer(s)	Alan Simpson

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0.1	2020-06-23	Initial draft	Lorna Smith
0.2	2020-07-07	Add training section	Juan Rodriguez Herrera
0.3	2020-07-13	Added eCSE	Chris Johnson
0.4	2020-07-13	Added CSE performance and metrics, outreach, publications	Xu Guo, Jane Kennedy, Lorna Smith
0.5	2020-07-13	Executive summary, future look, review	Lorna Smith
0.6	2020-07-13	Added details of I'm a Scientist Event (Outreach)	Jane Kennedy
0.7	2020-07-14	Added text for ARCHER2 Centralised CSE.	Xu Guo; George Beckett
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1. ARCHER Quarterly Report

This section of the report covers the period April 2020, May 2020 and June 2020 for the ARCHER2 service.

1.1 ARCHER Executive Summary

- The ARCHER eCSE programme has now finished. During the ARCHER service 222 proposals were received over 13 eCSE calls, leading to 100 awarded projects that funded 973 person months of effort. We had committed to awarding at least 941 person months by the end of the project (14 FTEs for 5 years, and 8.4 FTE for year 6) meaning 32 additional person months were awarded.

- The CSE team was heavily involved in testing, developing support documentation and supporting users as the ARCHER service returned to service after the recent security issue.

2. ARCHER Forward Look

- While the ARCHER service is due to be decommissioned when ARCHER2 comes into service, this is currently the main HPC resource for our users. Our focus over the next quarter is therefore on providing the best possible support to ARCHER users, until the service is decommissioned.

- We are also working to ensure that users transition successfully from ARCHER to ARCHER2 (see ARCHER2 report).

3. ARCHER Performance Report

This is the performance report for ARCHER CSE Service for the Reporting Periods: April 2020, May 2020 and June 2020.

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER 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	April 2020		May 2020		June 2020		Q2 2020	
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	100%	-1	100%	-1	100%	-3
FB1	100%	-2	-		-		100%	-2
Total		-7		-5		-5		-17

Service Credits

Period	April 2020	May 2020	June 2020
Total Service Points	-7	-5	-5

4. ARCHER CSE Queries

This section provides details on ARCHER CSE queries during the period April – June 2020.

Queries Resolved in Reporting Period

Metric Descriptions

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

A total of 39 queries were resolved by the CSE service in the reporting period.

Metric	Apr-20	May-20	June-20	Total
Technical Assessment: Grant	4	1	12	17
In-depth	4	1	6	11
Technical Assessment: Instant	3	3	2	8
Course Enquiry	0	1	0	1
Course Registration	1	0	0	1
eCSE Application	0	1	0	1
Total	12	7	20	39

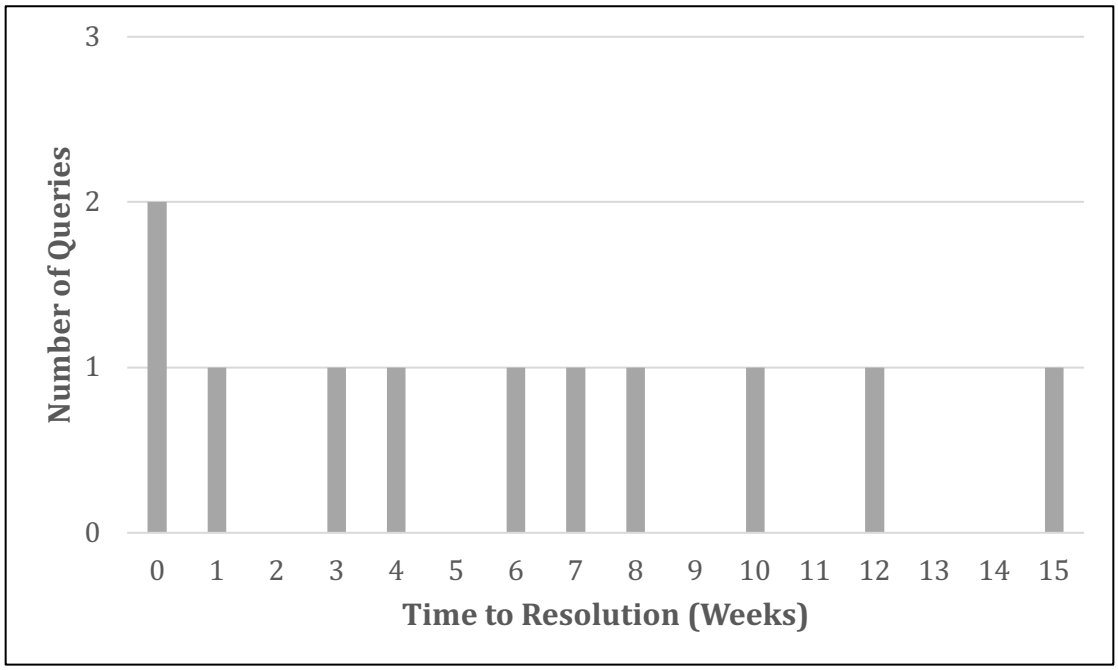
2 query feedback responses were received on In-depth queries in the reporting period. Both responses a score of “Excellent”.

Resolved In-Depth queries fell into the following categories:

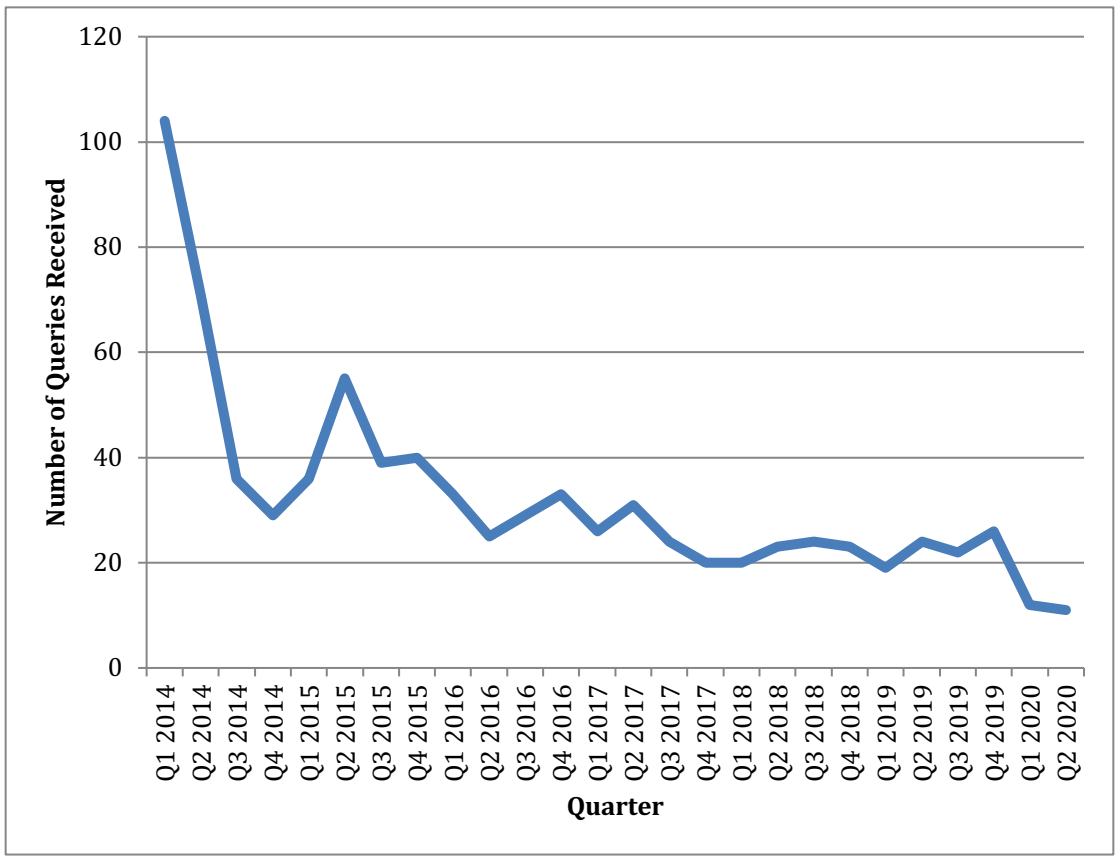
Category	Number of Queries	% Queries
3rd party software	9	81.8%
Compiler and system software	1	9.1%
User programs	1	9.1%

In-depth Query Analysis

The histogram below shows the time to resolution for In-Depth queries in the current reporting period.

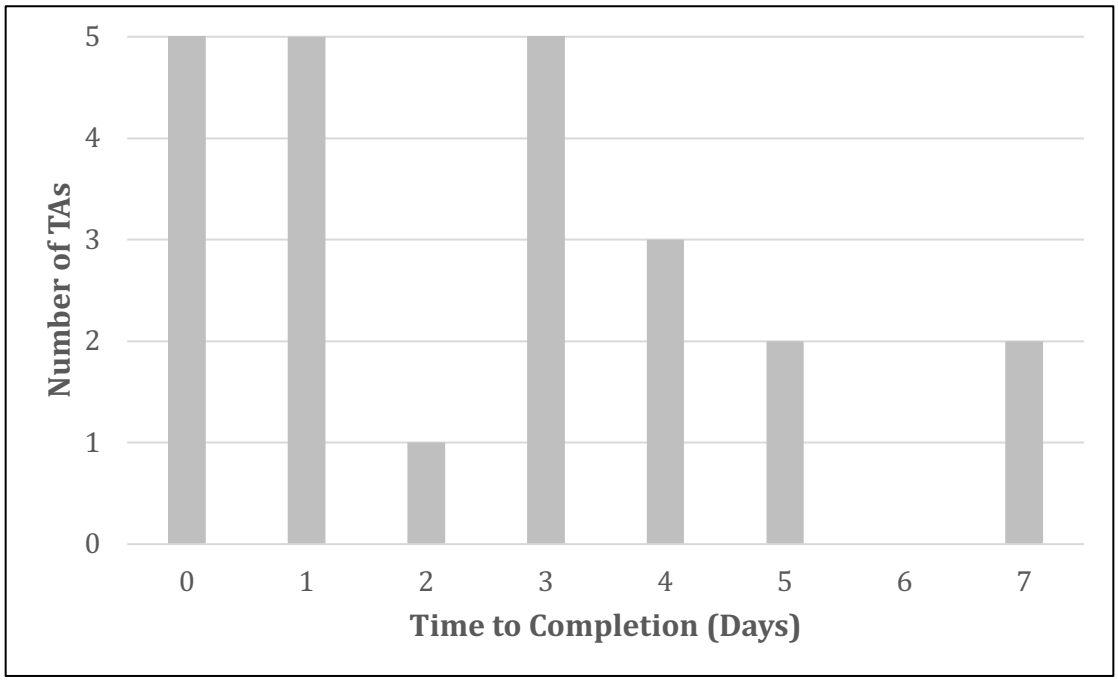


Plot of numbers of ARCHER In-Depth queries received per quarter:

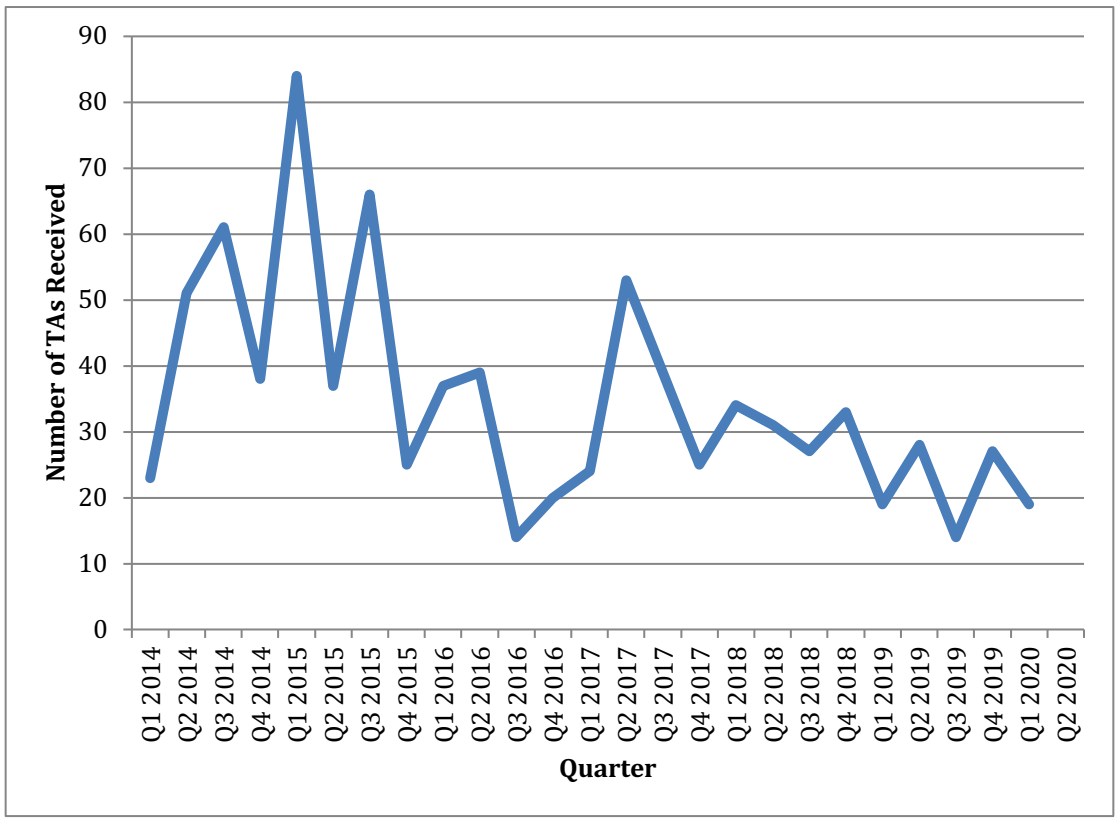


Technical Assessment Analysis

A histogram of the time to completion for ARCHER Technical Assessments is shown below.



Plot of numbers of ARCHER Technical Assessments received per quarter:



ARCHER 2 Quarterly Report

This section of the report covers the period April 2020, May 2020 and June 2020 for the ARCHER2 service.

5. ARCHER2 Executive Summary

- CSE
  - The CSE team have run a series of webinars providing an overview of the different aspect of the CSE service. This series has included material on the Service Desk, centralised support mechanisms, training and eCSE programmes and outreach activities. The team have also presented an overview of the ARCHER2 hardware and software environment.
  - The CSE team has access to the ARCHER2 TDS system and has been finalising user guides and documentation, finalising training course material and compiling and running application codes.
  - The CSE team is progressing two important service-improvement projects: one to evaluate popular software-management tools, to streamline and enhance the research-software catalogue for ARCHER2; and, the other to assess for users the impact of recent changes to the output management in the OpenFOAM CFD software.
- Training
  - A total of 13 days of online training have been delivered since April 2020, including virtual tutorials / webinars on a weekly basis. Online training courses have been very popular, with most courses oversubscribed.
  - The team ran a seminar on “Best Practice for Online Training” in early April. This provided best practice, experience and discussion of online training for the HPC Community during the early phases of Covid-19.
  - An external Training Panel has been formed, comprising representatives from the user community. This will provide independent direction to the training function. A draft curriculum and timetable for 2020/21 has been approved by this Training Panel.
- eCSE
  - The first ARCHER2 eCSE call opened on 19 May 2020 and closed for technical evaluations on 16 June 2020. 25 evaluations were carried out by the ARCHER2 CSE team.
  - The call then closed for proposals on 7 July 2020 receiving 25 proposals. This represents a significant number of applications. The panel meeting is expected to take place in late August or early September.
  - An independent eCSE panel has been formed, comprising a cross-section of representatives from the community.
- Outreach
  - Two members of EPCC staff participated in the I’m a Scientist event (https://imascientist.org.uk/). This involved online chats between both school groups and presenters that had planned to attend BBF, where students could ask scientists anything they like about their fields. This was a successful event with a lot of interaction, providing a reasonable alternative to the in-person activities cancelled due to Covid-19 (such as BBF).

6. ARCHER2 Forward Look

- Centralised
  - Having developed knowledge, expertise and documentation on the TDS, the next phase is to gain access to the 4-cabinet system (currently being installed in Edinburgh) and ensure the correct preparation is carried out before users gain access to the system.
  - The team will run a virtual tutorial / webinar for users describing experiences on the ARCHER2 TDS system.
- Training
  - Upcoming courses will be delivered online for the foreseeable future. Once the lockdown measurements are eased, we will investigate the timing of returning to our original plan to deliver face-to-face courses in several geographically distinct regions across the UK.
  - ARCHER2 specific courses, such as “ARCHER2 for software package users” and “Introduction to ARCHER2 for software developers” will be delivered once the ARCHER2 hardware is available. Internal runs of these courses will take place in July.
- eCSE
  - A provisional timetable of eCSE calls for the next year has been published on the ARCHER2 website.
  - For future calls we will be introducing a “Lightweight” eCSE programme. This gives PIs the opportunity to apply for projects requesting between 1-3 months, thus completing the spectrum of support between technical projects and full eCSE projects.
- Outreach
  - Due to the challenges of delivering outreach in person, the focus in the upcoming months will naturally be on developing online materials for the planned ARCHER2 Supercomputing Challenge, aimed at young people.

7. ARCHER2 Centralised CSE Team

In this section, we provide highlights from the CSE Team's work over the reporting period, focusing on topical service-improvement projects that are underway.

CSI Projects

Software management on ARCHER2 - Spack and EasyBuild

Maintaining a comprehensive catalogue of research software on a service like ARCHER2 is a challenging task. To simplify the task of keeping the catalogue up-to-date and to enable maximum domain coverage, we have undertaken an investigation into the capabilities and potential of two software-management tools, Spack and EasyBuild, to determine whether either could be used on ARCHER2 to help install and manage software packages.

Through testing on ARCHER, we found that both Spack and EasyBuild performed well and had potential to streamline the software-installation process for ARCHER2. By investing effort in the initial configuration, it is possible to create a near *turn-key* installation process, making it much easier to implement minor upgrades to existing packages and to redeploy or reconfigure software to meet changing user needs. Both Spack and EasyBuild also integrate well with common user-environment tools (module system), including both TCL Modules (as used on ARCHER) and the Lmod[1] system, which we plan to use on ARCHER2.

Ultimately, we decided that while both Spack and EasyBuild were found to be capable, EasyBuild's perceived greater stability, build reproducibility and ability to produce complete sets of build and install recipes (that can also be shared with others via, for example, GitHub) make it our preferred tool for ARCHER2.

We presented our findings from this project at an ARCHER2 virtual seminar (17th June 2020) (https://www.archer2.ac.uk/training/courses/200617-spack-easybuild/) and the CSE team has made contact with several other Supercomputing Centres who already use EasyBuild, with potential for future collaboration. At the time of writing, we are preparing to test EasyBuild on the ARCHER2 TDS system, to finalise a plan for deploying the tool onto the live service.

OpenFOAM new I/O model

OpenFOAM is a popular software package for running computational fluid dynamics (CFD) simulations on HPC systems such as ARCHER2. It has regularly featured in the top 20 most-used applications on ARCHER and will be part of the catalogue of centrally installed applications on ARCHER2.

One historical quirk of OpenFOAM is that it produces a very large number of output files: far more than other comparable applications. It is engineered to write a file per variable and per MPI-process when running in parallel on multiple processors. This has proved problematic for some power users, when running simulations on ARCHER (as for users of other peer HPC services), where the number of processors used is high and the number of files produced can quickly run into the 10,000s—100,000s (and clog up a user's file number quota).

In a recent release (v1706), the OpenFOAM developers have addressed this by adding an option to have all writing done to a single master file per variable, which can greatly reduce the total number of files generated. In this project, we are comparing the I/O performance of this new, collated writing method with the performance of the file-per-process method. Once complete, we will share the project's findings with ARCHER2 users and the wider CDF community, and update our documentation to highlight the recommended mode of use for OpenFOAM.

[1] https://lmod.readthedocs.io/en/latest/ — accessed 13th July 2020.

The I/O performance has been tested using a modified version of a common test case (the lid-driven cavity flow simulation). So far, tests of repeated simulations producing medium-sized output files have been carried out on 1, 2, 4, 8, 16, and 32 ARCHER nodes. We have observed that the uncollated (file-per-processor) output method begins to outperform the collated (file-per-simulation) method quite significantly when node-counts increased beyond eight. Simulations run using the 'collated' setting take nearly twice as long to run on 32 nodes, with I/O accounting for ~55% of the total simulation time, compared with less than 20% of simulation time in the 'uncollated' simulations.

Several further experiments will be conducted before drawing conclusions. We will compare results for larger output files and look at different write-strategies, attempting to reduce the I/O load of 'collated' mode.

An ARCHER2 virtual tutorial / webinar was delivered on 24th June 2020 based on the findings to date (https://www.archer2.ac.uk/training/courses/200624-openfoam-io/). All results will be available to ARCHER/ARCHER2 users once the project is fully completed.

8. ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from 6th May 2020 (ARCHER2 OCD) until end of June 2020. The performance report for ARCHER CSE Service is provided in Section 12 ARCHER Performance Report.

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER2 CSE Service Contract.

CSE Query Metrics

- **ARCHER2_CSE_Level1 (MTR)**: The Median Time to Resolution, as measured by Working Days (WDs), of all CSE queries falling within Level 1 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >4.4 WD; Operating Service Level: >1.4 WD, ≤2.4 WD.*
- **ARCHER2_CSE_Level2 (MTR)**: The Median Time to Resolution, as measured by Working Days (WD), of all CSE queries falling within Level 2 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >27 Working Days (WD); Operating Service Level: >12 WD, ≤17 WD.*
- **ARCHER2_CSE_Level3 (MTR)**: The Median Time to Resolution, as measured by Working Days (WD), of all CSE queries falling within Level 3 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >59 Working Days (WD); Operating Service Level: >29 WD, ≤39 WD.*
- **ARCHER2_CSE_TA (%):** The percentage of the total number of Technical Assessments (TAs) assigned to the Contractor in the Reporting Period completed prior to the commencement of the applicable TA Target Completion Date after the assignment of such Technical Assessment to the Contractor. *TA Target Completion Date in OY1: 8 WD; Service Threshold: <90.00%; Operating Service Level: 95.00-97.49%.*
- **Initial Response to Queries (%):** The percentage of the total number of CSE queries assigned to the Contractor in the Reporting Period responded to within 3 Working Hours. *Service Threshold: <96.00%; Operating Service Level: 98.00 – 98.99%.*
- **Query User Satisfaction (%):** The percentage of the total number of query satisfaction surveys completed in each Reporting Period, rating the quality of the resolution of Queries by the Contractor as "Good", "Very Good" or "Excellent". *Operating Service Level: 82.00 – 87.99%.*
- **Training User Satisfaction (%):** The percentage of all training satisfaction surveys completed in each Service Period, rating the Contractor as "Good", "Very Good" or "Excellent". *Operating Service Level: 88.00%-92.99%.*

Metric	May 2020 (starting from OCD)		June 2020		Q2 2020	
	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	0.1 WD	-2	0.1 WD	-2	0.1 WD	-4
ARCHER2_CSE_Level2 (MTR)	4.6 WD	-2	4.7 WD	-2	4.7 WD	-4
ARCHER2_CSE_Level3 (MTR)	-		-		-	
ARCHER2_CSE_TA (%)	-		100%	-1	100%	-1
Initial Response to Queries (%)	100%	-1	100%	-1	100%	-2
Query User Satisfaction (%)	100%	-2	100%	-2	100%	-4
Training Satisfaction (%)	95.7%	-0.25	100%	-1	97.4%	-1.25
Total		-7.25		-9		-16.25

17 *query feedback* responses were received on query resolution in the Reporting Period. 100% of responses had a score of "Good", "Very Good" or "Excellent".
39 *training satisfaction* responses were received in the Reporting Period. 97.4% of responses had a score of "Good", "Very Good" or Excellent". There was a single "Bad" response.

9. ARCHER2 CSE Queries

This section provides details on ARCHER2 CSE queries during the Reporting Periods from 6th May 2020 (ARCHER2 OCD) until end of June 2020period April – June 2020.

CSE Query Statistics

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER2 CSE Service Contract.

- **No. of Assigned:** The number of CSE queries assigned to the Contractor within each query resolution category in the Reporting Period.
- **No. of Resolved:** The number of CSE queries resolved by the Contractor within each query resolution category in the Reporting Period.
- **Backlog:** The number of CSE queries assigned to the Contractor that remained unsolved within each query resolution category in the Reporting Period
- **Avg No. of Correspondence:** The average number of pieces of correspondence generated for CSE queries in each query resolution category.
- **Avg Time of First Responses:** The average time taken for the Contractor to first respond to the Originator of the CSE query.

A total of 170 queries were resolved by the ARCHER2 CSE service in the Reporting Period. Please note during the preparation phase before ARCHER2 OCD (i.e. from April until 5th May), 97 ARCHER2 CSE queries have been resolved and 11 queries were continued for resolution after the ARCHER2 OCD.

May 2020 (from OCD)					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	80	89	1	5	0.6 hrs
ARCHER2_CSE_Level2	5	2	4	18	1.3 hrs
ARCHER2_CSE_Level3	-	-	-	-	-
ARCHER2_CSE_TA	-	-	-	-	-
June 2020					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	40	40	1	5	0.4 hrs
ARCHER2_CSE_Level2	40	38	6	10	0.6 hrs
ARCHER2_CSE_Level3	-	-	-	-	-
ARCHER2_CSE_TA	1	1	0	8	1.6 hrs
Q2 2020 (from OCD)					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	120	129	1	5	0.5 hrs
ARCHER2_CSE_Level2	45	40	6	10	0.7 hrs
ARCHER2_CSE_Level3	-	-	-	-	-
ARCHER2_CSE_TA	1	1	0	8	1.6 hrs

CSE Query Categories

Resolved CSE queries in the Reporting Period fell into the following categories:

Service Level	Category	Number of Queries	% Queries
ARCHER2_CSE_Level1	Courses	128	75.3%
	Compilers and system software	1	0.6%
ARCHER2_CSE_Level2	eCSE Applications/Calls	27	15.9%
	Access to HPC	7	4.1%
	Courses	3	1.8%
	Login, passwords and ssh	2	1.2%
	Compilers and system software	1	0.6%
ARCHER2_CSE_TA	UKRI Fellowship	1	0.6%
Total		170	100%

10. ARCHER2 Training

As part of ARCHER2, the service has been developing and delivering a training programme for the ARCHER2 community. The training plan for the upcoming year (May 2020 – April 2021) was approved by an external Training Panel on 12th May.

Since April, the CSE service has provided a total of 13 days of online training, scheduled as follows:

Dates	Course	Days	Attend
8 April 2020	Best Practices for Online Training	0.5	66
15 April 2020	ARCHER2 Overview - A Service for Users	0.5	45
22 April 2020	Introduction to the ARCHER2 hardware and software	0.5	104
29 April 2020	Porting and performance of DiRAC HPC benchmarks on Oracle bare metal cloud	0.5	22
4, 11, 25 May 2020	LAMMPS	1.5	34
6 May 2020	ARCHER2 Training	0.5	23
13 May 2020	ARCHER2 Spectrum of Support	0.5	19
14-15, 29 May 2020	Message-passing programming with MPI	3	28
20 May 2020	The determination of clusters structures combining infrared spectroscopy and DFT calculations	0.5	24
27 May 2020	ARCHER2 eCSE	0.5	24
3 June 2020	ARCHER2 Outreach	0.5	17
9 June 2020	Preparing to run biomolecular QM/MM simulations with CP2K using AmberTools	0.5	19
10 June 2020	ExCALIBUR - an algorithmic approach to exascale design	0.5	125
17 June 2020	Software Packages in HPC with Spack and EasyBuild	0.5	72
24 June 2020	A review of OpenFOAM collated I/O performance on ARCHER	0.5	34
29-30 June 2020	HPC Carpentry	2	20

A weekly programme of virtual tutorials / webinars started on 8th April. Given the current lack of face-to-face courses due to coronavirus lockdown rules advised by the UK government, we increased the delivery frequency of virtual tutorials / webinars from monthly to weekly in order to reach a larger audience. This has already proved successful, with two recent virtual tutorials / webinars attracting more than 100 attendees. The Blackboard Collaborate system, which we will use for all online training, was comfortably able to accommodate this number.

On the feedback for online courses, attendees rate the course on a scale of 1-5 (“Very Bad”, “Bad”, “Good”, “Very Good” and “Excellent”). The average feedback using this metric was 4.46, i.e. better than “Very Good”. Users provided 39 feedback forms, a response rate of 48%

11. ARCHER2 The Embedded CSE Programme (eCSE)

As part of ARCHER2, the CSE service will deliver an eCSE programme to provided distributed CSE support across the UK. The first call received 25 proposals from a broad range of subject areas with PIs from 15 different UK Institutions. A total of 235 Person-Months of effort has been requested from 13 different UK institutions. A panel of 15 experts has been formed, a subset of whom will assess the proposals at the panel meeting in August/September, with projects expected to start later in the year. This coincides with the start of the ARCHER2 service.

12. ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Community Engagement and Impact

Alan Simpson presented a talk at the RSE Leaders Meeting (virtual/Zoom) on the 19 June 2020. This gave an overview of the ARCHER2 service, covering training, outreach, the eCSE and engagement with the RSE community. The talk provided an opportunity for us to explain the ARCHER2 service to RSE leaders and gain feedback and discussion.

Outreach Activities and Events

Two of the three large science festivals EPCC committed to attend each year for outreach were to take place in March/April: Big Bang UK Young Scientists and Engineers Fair (BBF) in Birmingham, and Edinburgh Science Festival (ESF). Due to the size and hands-on nature of these events, both were cancelled in response to the spread of COVID-19.

In place of the physical events, EPCC contributed to online alternatives. The *I'm a Scientist* organisation (https://imascientist.org.uk/) hosted online chats between both school groups and presenters that had planned to attend BBF, where students can ask scientists anything they like about their fields. Two members of EPCC staff participated in this event. ESF moved entirely online, and existing materials from the ARCHER website were provided. Due to the online nature of this year's ESF, all festival materials continue to be available, and ARCHER materials can be found here: https://www.sciencefestival.co.uk/event-details/an-introduction-to-supercomputing.

Planning future events continues to be a challenge due to the uncertainty over COVID-19, however a proposal has been submitted to The Big Bounce Festival of Physics, due to take place in November. One of the aims of this festival is to raise the profile of work by scientists from under-represented groups in physics/STEM.

Due to the challenges of delivering outreach in person, focus in the upcoming period will naturally continue on developing online materials for the planned ARCHER2 Supercomputing Challenge, aimed at young people. Currently, this is at the requirements/planning stage: the primary aim is to make something that is inclusive to anyone: that is, there are no dependencies on specific items such as arts and craft supplies or a printer, that might introduce a barrier to people taking part.

A repository of outreach materials is being added to the ARCHER2 website at: https://www.archer2.ac.uk/community/outreach/materials/.

Presentations, Publications and Outputs

The following is a list of all presentations, meetings, exhibitions and outreach events carried out by the CSE team to support the ARCHER2 service. Due to Covid-19, travel to events has been restricted and many events have been cancelled. However, some events and meetings were held online. The following is a list of online events attended by the team.

- Alan Simpson, RSE Leaders Meeting (virtual/Zoom), 19 June 2020. Presented a talk on "ARCHER2: Training, eCSE, Outreach and the RSE Community".
- Juan Rodriguez Herrera, SIG IO UK Meeting. 23 April, 2020.
- Juan Rodriguez Herrera, Virtual Workshop: Toward a Globally Acknowledged and Free HPC Certification, 4 May 2020.
- Juan Rodriguez Herrera, ISC High Performance, 2020. 22-25 June, 2020.

- Juan Rodriguez Herrera, ICS-2020 (the 34th ACM International Conference on Supercomputing). 29 June - 2 July, 2020.
- Andy Turner, Materials and Molecular Modelling Exascale Working Group Kickoff Workshop, 11 May 2020, Online.
- Andy Turner, George Beckett and Alan Simpson, ARCHER2 Virtual Factory Acceptance test, 23-25 June 2020, Online.
- Jane Kennedy and Oliver Brown, I'm a Scientist, Stay at Home! Science Week Zone. Online instant messaging chats with classes from various schools, 11th-13th March.