



ARCHER CSE Service Quarterly Report

Quarter 1 2020



1. Document Information and Version History

Version:	1.0
Status	Release
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Reviewer(s)	Alan Simpson

Version	Date	Comments, Changes, Status	Authors, contributors, reviewers
0.1	07-04-2020	Skeleton document	Lorna Smith
0.2	15-04-2020	Content added eCSE, CSI, Training	Chris Johnson, Xu Guo, David Henty, George Beckett
0.3	15-04-2020	Document review, additional content added, full draft completed	Lorna Smith
0.4	16-04-2020	Reviewed	Alan Simpson
1.0	16-04-2020	Version for UKRI	Lorna Smith, Alan Simpson

2. Executive Summary

This report covers the period: 1 January 2020 to 31 March 2020 inclusive.

- Covid-19
 - Covid-19 has resulted in significant changes to everyone's daily lives and has impacted on a large number of services across the country. The ARCHER CSE team have smoothly transitioned to working from home, with no impact on the service offered to our users. Recent BCDR scenario tests proved their value, with robust procedures in place to handle remote operation and significant sickness.
 - The CSE team have been supporting the HEC BioSim consortium to set up and implement a short-notice call for computing projects on ARCHER (and EPSRC Tier-2 services) for research and development targeted at addressing the ongoing Covid-19 pandemic.
 - The service is currently running weekly webinars and plan to continue this for at least the next 3 months. The aim is to engage with the user community, providing continuity and visibility during this time.
- Centralised CSE Team:
 - The CSE team has completed a final review of the large portfolio of scientific software on ARCHER, including end-user applications, underlying libraries, and supporting tools. This will inform decisions about scientific-software provision on ARCHER2.
 - The enhanced Service Desk for ARCHER2 has been provisioned from the beginning of April. A combined ARCHER-ARCHER2 team now handles all CSE-related queries, paying particular attention to adjustments and provisions that need to be made for the transition to ARCHER2.
 - New contacts have been identified for the Consortium contacts role on ARCHER2 and contact has been made with Consortium representatives. This is to ensure the specific requirements of the Consortia are understood and addressed on ARCHER2.
- eCSE:
 - All eCSE projects have now completed and the last 2 final reports are due imminently. Work continues to add project highlights to the ARCHER web site; these highlights demonstrate the breadth and success of the eCSE programme.
- Outreach and Engagement:
 - Covid-19 has impacted on the work of the Outreach team, with both the Big Bang Fair (BBF) and the Edinburgh International Science Festival (EISF) understandably cancelled during this difficult time. Alternative online events have been organised around BBF and EISF and the team have participated in these.
- Training:
 - We delivered the final 7 days (120 student-days) of face-to-face training before the closure of the training programme in February. These were at 3 different locations (with an average feedback score better than "Very Good"). In addition, there was 1 day (7 student-days) of live-broadcast online training. Together with 1.5 day of online tutorials, this meets this quarter's pro-rata target of 9.5 days.
 - To help users in the transition to ARCHER2 we ran two virtual tutorials covering: how best to transfer data from ARCHER; and new features of the Cray Compilers.

3. Collaborations and Outputs Summary

Covid-19 has understandably led to a number of restrictions and cancellation of events. A small number of physical events have been replaced by virtual events.

- Presentations:
 - A. Simpson, “ARCHER2 Update”, HPC Champions, Bath, 26th February, 2020.
- Meetings:
 - J. Beech-Brandt, HPC-SIG, Bath, 25th February, 2020.
- Exhibitions and Outreach Events:
 - J. Kennedy “I’m a Scientist”, Science Week 2020, 11-13th March. Online Q&A session (developed in response to the cancellation of the Big Bang Fair).
 - “An Introduction to Supercomputing”, Edinburgh International Science Festival digital alternative due to Covid-19, 4th – 19th April, online resources: <https://www.sciencefestival.co.uk/event-details/an-introduction-to-supercomputing>

4. Forward Look

- Centralised CSE Team:
 - The delay to the availability of ARCHER2 hardware has led to an extension of the existing ARCHER service. Over the coming months we will focus on delivering the best possible service to our ARCHER users, maintaining this service through until ARCHER is turned off.
 - The service will continue to support the HEC BioSim consortium with the set up and implementation of computing projects on ARCHER targeted at addressing the on-going Covid-19 pandemic.
 - The service will continue to adapt and to support users during the unusual circumstances surrounding Covid-19. Weekly webinars will help to maintain links with the user community.
 - ARCHER2 planning and implementation is well underway, and this will continue to ensure the CSE service is ready to support users once the ARCHER2 hardware is available.
- eCSE:
 - No further eCSE calls are planned under ARCHER, but the programme re-appears under ARCHER2. The first ARCHER2 eCSE call is due to open on the 19th May 2020. This should allow successful projects to start work on the ARCHER2 service as soon as the hardware is available.
- Outreach
 - Covid-19 has understandably seen a number of outreach events cancelled, such as BBF and EISF. This is anticipated to continue for some time. However there is greater interest in online resources and the teams focus will be on enhancing our online offering to meet this need.
- Training:
 - No further training is planned under ARCHER, but the programme will continue under ARCHER2 with a range of new courses to meet the needs of the user community. For the initial period, these are expected to be online, live-broadcast courses.

5. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: January 2020, February 2020 and March 2020.

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 Metric	Jan-20		Feb-20		Mar-20		Q1 2020	
	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	100%	-2	100%	-6
Total		-7		-7		-7		-21

Training Metrics

- FB2:** The percentage of all training satisfaction surveys (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	Jan-20		Feb-20		Mar-20		Q1 2020	
	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
FB2	100%	-1	100%	-1	100%	-1	100%	-3
Total		-1		-1		-1		-3

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

Service Credits

Period	Jan-20	Feb-20	Mar-20
Total Service Points	-8	-8	-8

6. 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
Course Enquiry	Enquiries about courses
Technical Assessment: <Category>	Request for Technical Assessments of applications for ARCHER time
eCSE Application	Queries relating to eCSE applications

A total of 83 queries were resolved by the CSE service in the reporting period.

Metric	Jan-20	Feb-20	Mar-20	Total
Course Registration	34	19	1	54
In-depth	3	4	2	9
Course Enquiry	2	0	1	3
Technical Assessment: Grant	5	3	3	11
Technical Assessment: Instant	1	1	2	4
Technical Assessment: RAP	0	0	1	1
eCSE	1	0	0	1
Total	46	27	10	83

No query feedback responses were received on In-depth queries in the reporting period.

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd party software	5	55.6%
Compiler and system software	3	33.3%
User programs	1	11.1%

In-Depth Query Highlights

One In-Depth query has been selected to illustrate the work of the centralised CSE team over the reporting period. The number of in-depth queries has been relatively low during this period, we believe partly due to the anticipated end of the ARCHER service in February and also due to the significant disruption caused by Covid-19.

Q1303636 in-situ visualisation - ARCHER

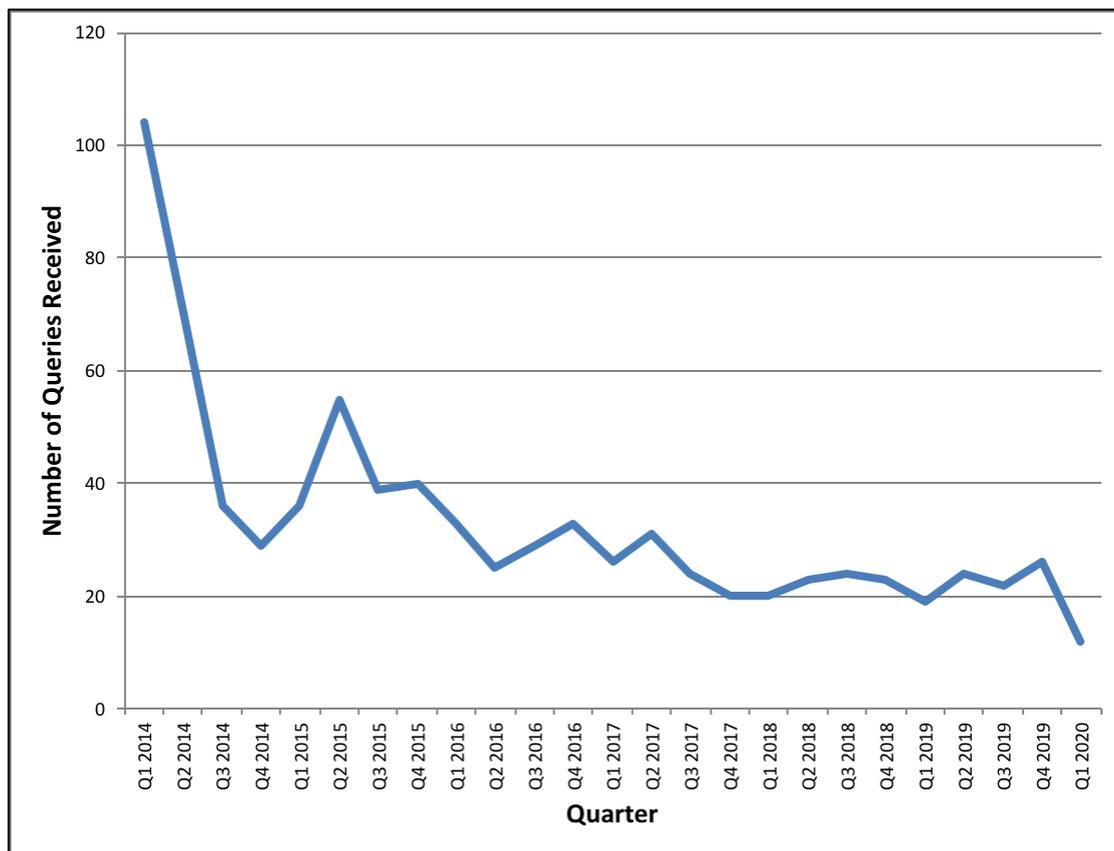
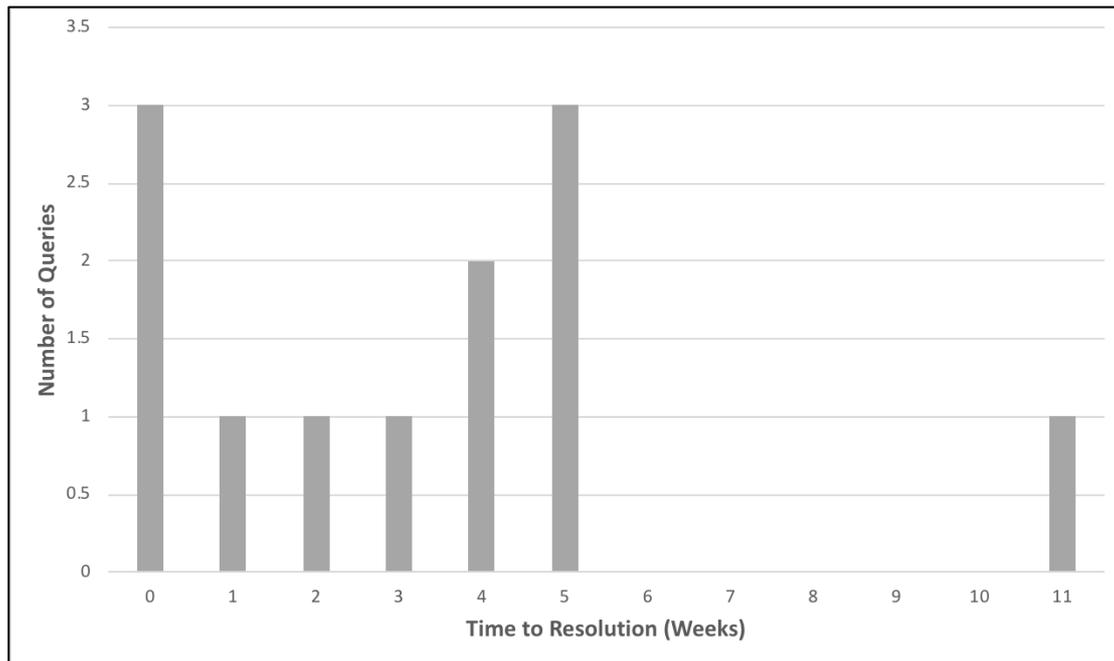
In this query a user was looking to use Paraview for in-situ visualisation and to install Catalyst. We advised that this isn't possible on ARCHER, but offered the UK_RDF DAC as an alternative, providing guidance on what could and could not be done on ARCHER and the UK_RDF DAC. The user was able to install Catalyst and Paraview. Following a discussion, the user has offered to install Paraview on ARCHER2, once the system is up and running.

This query is a good example of impact of the transition period between ARCHER and ARCHER2, with preparation work completed on the existing service to ensure software can be installed on the new ARCHER2 system quickly.

In-Depth Query Analysis

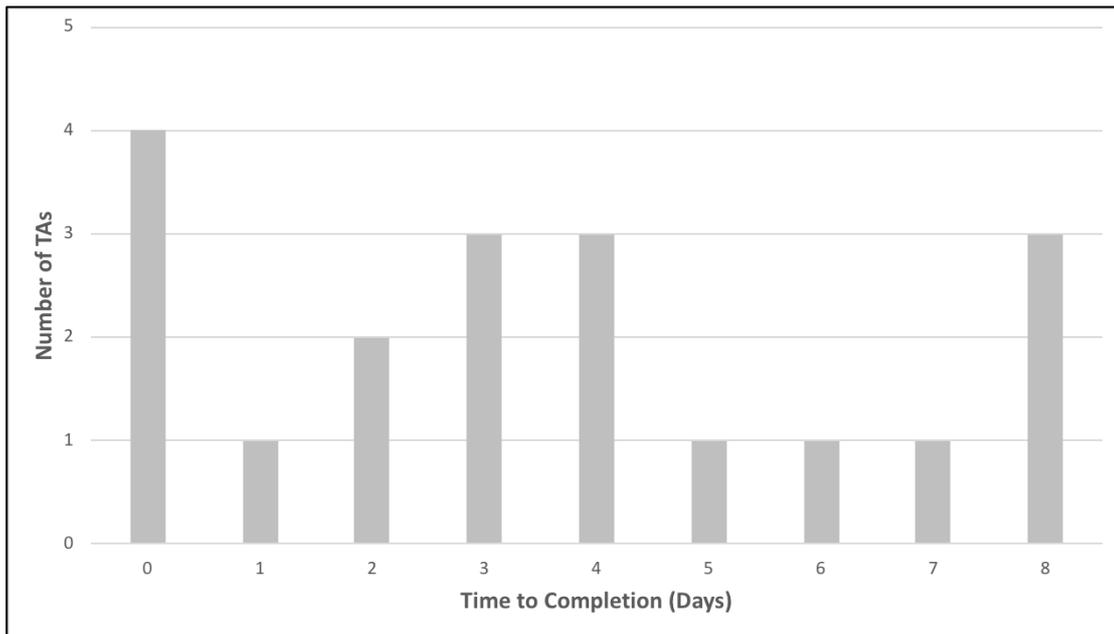
The histogram below shows the time to resolution for In-Depth queries in the current reporting period.

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

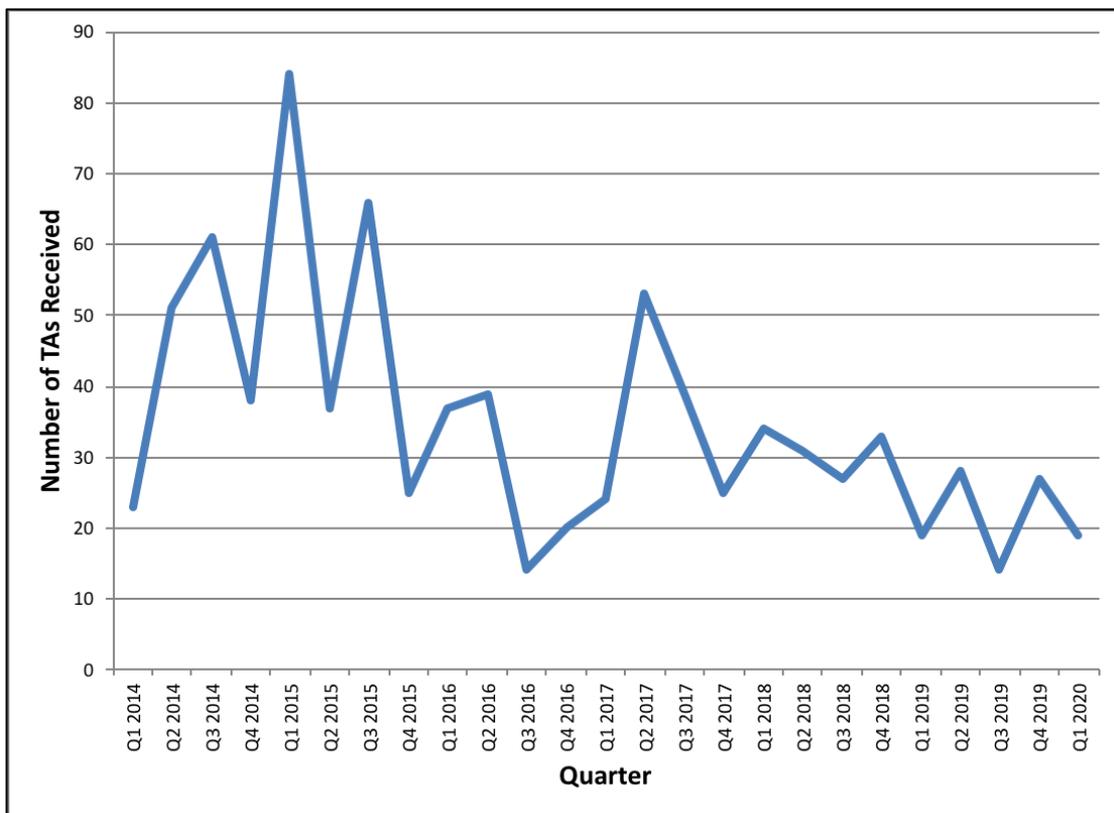


Technical Assessment Analysis

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



Plot of numbers of Technical Assessments received per quarter:



7. Centralised CSE Team: Continual Service Improvement

In collaboration with user groups and the other Service partners, the CSE service identified several priority service improvement areas, including those for the future national service ARCHER2, to invest technical effort from the centralised CSE team. This section provides highlights from the reporting period.

Containers for HPC

Following on from our previous report after our successful installation and running of RAMSES code with containers on Cirrus, we are in the process of setting up a Singularity container to run a set of ARCHER benchmark codes on Cirrus, including CASTEP, CP2K and GROMACS. We plan to compare the performance gained using the Singularity container with their “bare metal” results tested without any container. In addition, we have been investigating the use of Singularity containers on other HPC systems such as CSD3, and plan to compare these results with our previous experience and with results from Cirrus.

Frameworks for Building and Managing Packages on ARCHER2

With the impending launch of ARCHER2 we have examined how the scientific software packages to be provided to users might be installed and managed.

Spack and EasyBuild are two HPC-oriented build systems. We have examined the difference in philosophy between the two frameworks and also considered the advantages and disadvantages they bring when compared to a more traditional manual installation method. Of particular interest is how these frameworks can expedite and simplify the process of building and installing a reproducible software stack. Part of the analysis was carried out using ARCHER as an ARCHER2 substitute. The work is currently being written up and a whitepaper will be made available to ARCHER/ARCHER2 users.

Spack (<https://github.com/spack/spack>)

EasyBuild (<https://easybuilders.github.io/easybuild/>)

8. Training

Up to the close of the training service in February, the CSE service has provided 7 days (120 student-days) of face-to-face training across 3 different locations, 1 day (7 student-days) of live-broadcast online training and 1.5 days of online tutorials (average attendance 15 per tutorial).

Month	Dates	Course	Location	Days	Attend
Jan 2020	7-8	Hands-on Introduction to HPC	Edinburgh	2	18
	9-10	GPU Programming with CUDA	Edinburgh	2	21
	15-22	Using Non-Volatile Memory	Online	1*	7
	27-28	Advanced MPI	London	2	16
	29	Transferring Data from ARCHER	Online	0.5	
Feb 2020	3	Reproducible Computational Environments using Containers	Durham	1	10
	5	Cray Compilation Environment	Online	0.5	
	12	EIS-2: General Purpose High Performance Input & Maths Parser	Online	0.5	

* This online interactive course was run over two consecutive Wednesday afternoons, giving time for attendees to attempt the practical exercises between sessions and to raise any issues with the trainer at the second webinar.

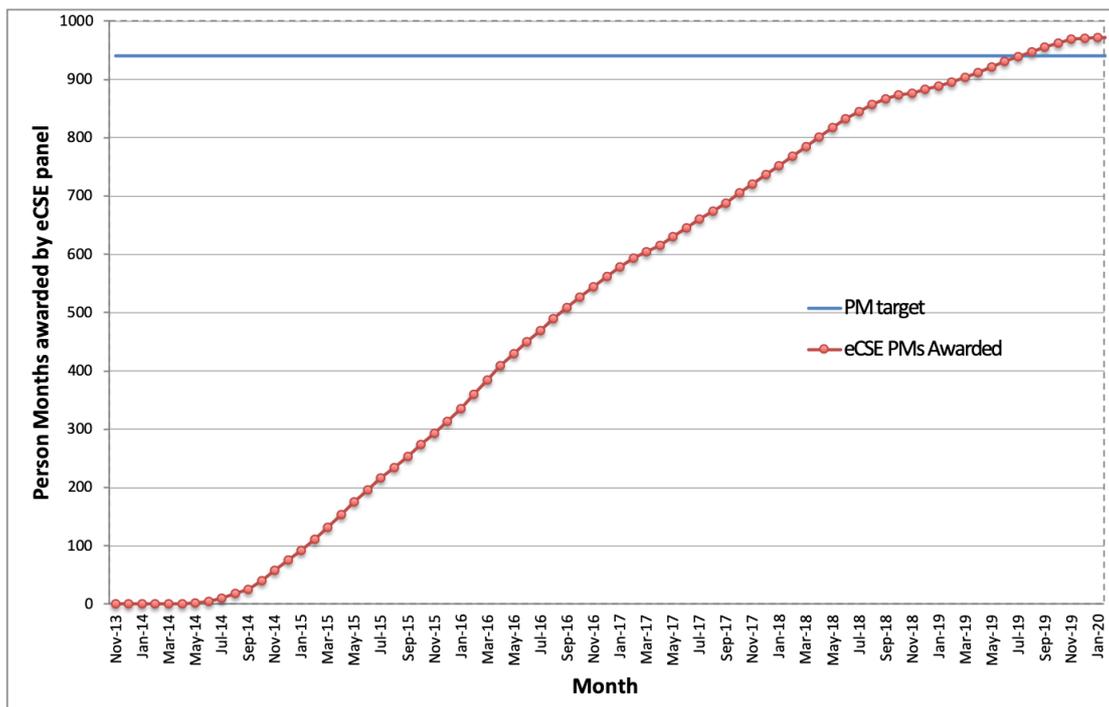
On the feedback for face-to-face courses, attendees rate the course on a scale of 1-5 (“Very bad”, “Bad”, “Good”, “Very good” and “Excellent”). The average feedback using this metric was 4.3, i.e. better than “Very Good”. Users provided 34 feedback forms, a response rate of 52%.



9. CSE (eCSE)

Overview of eCSE Effort

All eCSE projects have now completed. Two final reports are still outstanding, but due to be completed shortly. Of the 100 projects, 95 have submitted final reports, 2 are outstanding but due shortly, 1 has not been completed due to personal circumstances, and 2 have failed to submit.



- The eCSE person months awarded up to and including the 13th eCSE call are shown in red.
- We committed to awarding at least 941 person months by the end of the project (14 FTEs for 5 years, and 8.4 FTEs for year 6).
- 973 person months have been awarded across 100 eCSE projects, meaning an extra 32 person months have been awarded over the programme.

eCSE call	No. proposals	No. projects awarded	No. person months awarded	No. projects started	No. projects completed	No. final reports received	Notes
eCSE01	19	14	132	14	14	14	
eCSE02	17	9	82	9	9	9	
eCSE03	16	10	96	10	10	10	
eCSE04	16	8	82	8	8	8	
eCSE05	14	8	94	8	8	8	
eCSE06	9	5	47	5	5	5	
eCSE07	16	5	49	5	5	5	
eCSE08	21	8	88	8	8	8	
eCSE09	19	5	58	5	5	4	1 final report has not been received and

							will no longer be chased.
eCSE10	13	6	59	6	6	6	
eCSE11	18	6	49	6	6	4	2 final reports have not been received and will no longer be chased.
eCSE12	23	6	41	6	6	6	
eCSE13	21	10	96	10	10	8	2 late final reports are being pursued.
Total	222	100	973	100	100	95	

10. ARCHER to ARCHER2 Transition

New contacts have been identified for the Consortium Contacts role on ARCHER2. These contacts have introductions to the relevant Consortia and (as well as being the point of contact for ARCHER2 matters) and will field enquiries and requests related to ARCHER through to the end of service.

We have been supporting the HEC BioSim consortium to set up and implement a short-notice call for computing projects on ARCHER (and EPSRC Tier 2 services) for research and development targeted at addressing the ongoing Covid-19 pandemic.

A set of initial documentation for ARCHER2 has been defined and is in progress. This will include practical guidance on how to transition applications and workflows from ARCHER to ARCHER2.

The Service Desk for ARCHER2 has been provisioned and staffed from the beginning of April. A combined ARCHER-ARCHER2 team will be handle all CSE-related queries from ARCHER, from this point on, paying particular attention to adjustments and provisions that need to be made given the future transition to the new service and the impact that will have on queries we receive.

The CSE team maintains a large portfolio of scientific software on ARCHER, including end-user applications, underlying libraries, and supporting tools. The CSE team has completed a final review of the software catalogue, to inform decisions about scientific-software provision on ARCHER2 and help identify any potential issues (e.g., incompatibility) that may affect the computational-science community.