ARCHER and ARCHER2 Quarterly Report

April – June 2021

EPCC

The University of Edinburgh

1. Document Information and Version History

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0.2	2021-06-04	eCSE info added	Chris Johnson
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ARCHER 2 Quarterly Report

This section of the report covers the period April 2021 – June 2021 for the ARCHER2 service.

2. ARCHER2 Executive Summary

- The CSE team have recently gained access to the full system and are currently testing a range of applications, tools and libraries to ensure the system is appropriate for user service.
- The level of CSE queries on the 4CAB system has decreased to a more typical level (compared to the high volume seen in the previous period). This has allowed the CSE team to focus on improvement projects, such as a review and update of existing documentation.
- The CSE team is collaborating with one of the PRACE-6IP activities to develop best practice guides for ARCHER2 users on the optimal running conditions for different applications.
- During this period the training team ran a virtual tutorial on Python and six courses, which includes an advanced ARCHER2 course taught by HPE Cray, making a total of 12.5 training days.
- The CSE team was involved in running two ISC'21 sessions dedicated to online HPC education and training. The first one was a Birds of a Feather session and the second a workshop session. These highlighted the opportunities associated with online learning platforms and methodologies, such as increased accessibility and inclusivity, compared to in-person alternatives.
- Four eCSE calls have now been run with 35 projects having been awarded a total of 318 person months (PMs). This includes projects from the most recent (fourth) call where the panel meeting took place on 29 June 2021 awarding 7 projects a total of 60 PMs.
- eCSE calls 2-4 included both the EPSRC and NERC remits with 62 PMs available to NERC projects and 514 PMs available to EPSRC projects. All of the 62 NERC PMs have now been awarded meaning that from call 5 onwards proposals will be invited for software within the EPSRC remit only.
- A series of 8 blog articles have been published providing details of the ARCHER2 service, some of the research software on it, and highlighting user scientific research.
- ISO 9001/27001 - Work is underway to prepare for our ISO 27001 information security re-certification audit which is due in September 2021. We have an annual ISO 9001 quality annual surveillance audit at the same time. These audits help ensure the quality of the services we deliver meet and exceed requirements.
- 130 feedback responses have been received from 622 total CSE queries, with the majority of the feedback sitting in the excellent or very good category.
- A donation of £1 per user feedback response has been made to our selected charity, Save the Children. This quarter a total donation of £253 has been made, with £130 from the CSE Query feedback.
- The ARCHER2 service has been accepted for the University of Edinburgh's Images of Innovation Exhibition at the UN Climate Change Conference (COP26). In addition to an image of the service, there is information on the service and its approach to equality diversity and inclusion.

3. ARCHER2 Forward Look

- As the full system progresses towards user service, the CSE team will work closely with all service partners to ensure that the service is ready for users.
- The CSE team will continue to focus on supporting the 4CAB system, which is the visible part of the service to users.
- This quarter will see a set of new courses being delivered, covering topics such as C++, advanced MPI, and performance tools. We are also working on increasing the number of self-service courses. Virtual tutorials on software packages available on ARCHER2 will also be scheduled once the summer period is over.
- As part of our commitment to encouraging and developing Early Career Researchers, selected observers are invited to attend and observe an eCSE panel meeting to give them a better insight into this competitive selection process to assist in the preparation of funding proposals. Following on from last year's very successful call for early career observers a further call will be run alongside the eCSE05 call later this year.
- The series of blog articles have proved popular and we plan to continue to publish a regular set of these, with future articles around the anticipated queue setup on ARCHER2, and performance and benchmarking on the full ARCHER2 system.
- We will have our annual ISO 9001 and 27001 external audits in September this year. An approved external auditor will spend a week with us reviewing our quality and information security processes and policies.
- As part of our commitment to mentor and enhance the career opportunities of Early Career researchers, CSE staff are active in planning for the International HPC Summer School (IHPCSS). CSE staff members will be involved in teaching one of the tracks, running the mentoring programme, organising the programming challenge, and creating the virtual instance for the social and mentoring activities. The organisers are applying various tactics to ensure the all-online format still creates an inclusive, interactive and engaging opportunity for students to learn more about HPC, and to interact with their peers and mentors.

4. ARCHER2 Centralised CSE Team

During this period, the CSE service has run smoothly with a more typical level of user queries, compared to the high volume seen in the previous period. Alongside the usual contributions to good service, this allowed CSE staff to invest effort in various service improvements, including:

- Extensions to the ARCHER2 Documentation website, to include topics on data analysis and tools (specifically, R statistics and Visidata).
- Testing and documenting an update to the Cray Programming Environment (Version 21.03) which included important fixes for problems identified during early-life support and also brought the 4-cabinet system into line with the expected programming-environment configuration for the main system.
- Given the change to the timeline for transitioning to the main system, the CSE team contacted potentially impacted HEC Consortia to ensure they were able to get maximum use from the 4-cabinet interim system.
- Finally, the CSE team has been preparing for access to the main system, to ensure we can quickly contribute to validation work, update supported applications for the increased capacity of the main system, plus update best-practice guides and other documentation.

CSI Projects

The CSE team has been involved in several service-improvement projects during the reporting period:

- The team has been measuring the performance of the quantum chemistry application (CP2K), focusing on the QM/MM model, which is critical to a wide range of high-end simulations. Work has used both the ARCHER2 4-cab service and, for comparison, the Cirrus Tier-2 service. Findings from the work informed the QM/MM training course, which was run in April, using a CSE-provided configuration of the Gromacs + CP2K interface code.
- The CSE team is collaborating with one of the PRACE-6IP activities to benchmark and optimise the performance of several centrally supported candidate codes based on the ARCHER2 4-cabinet system. This will result in best practice guides for ARCHER2 users on the optimal running conditions as well as providing general advice on optimising the performance of different compilers and libraries available on ARCHER2.
- Continuing the work reported in the previous quarter, the team has demonstrated that the nanoscale molecular dynamics application, NAMD, scales scale very well on the ARCHER2 4-cabinet system, using test cases of up to 210-million atoms. Better still, this performance was realised with little in the way of application-specific tuning, suggesting that the default configuration is well tuned. In the coming period, we will extend the work to other candidate codes, validate our results on the main system, and compare to Tier-0 systems available through the PRACE network.

5. ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from April 2021 until end of June 2021.

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	April 2021		May 2021		June 2021		Q2 2021	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	0.1WD	-2	0.1WD	-2	0.1WD	-2	0.2WD	-6
ARCHER2_CSE_Level2 (MTR)	0.1WD	-2	0.2WD	-2	0.5WD	-2	0.3WD	-6
ARCHER2_CSE_Level3 (MTR)	27WD	-0.5	23WD	-0.5	-		25WD	-1
ARCHER2_CSE_TA (%)	100%	-1	100%	-1	100%	-1	100%	-3
Initial Response to Queries (%)	100%	-1	99.4%	-0.25	100%	-1	99.8%	-2.25
Query User Satisfaction (%)	98.1%	-2	97.1%	-2	97.6%	-2	97.7%	-6
Training Satisfaction (%)	100%	-1	100%	-1	100%	-1	100%	-3
Total		-9.5		-8.75		-9		-27.25

130 query feedback responses were received on query resolution in the Reporting Period. 97.7% of responses had a score of “Good”, “Very Good” or “Excellent”.

6. ARCHER2 CSE Queries

This section provides details on ARCHER2 CSE queries during the Reporting Periods from April 2021 until end of June 2021.

CSE Query Statistics

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

- **Assigned:** The number of CSE queries assigned to the Contractor within each query resolution category in the Reporting Period.
- **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
- **Correspondence:** The average number of pieces of correspondence generated for CSE queries in each query resolution category.
- **First Response:** The average time taken for the Contractor to first respond to the Originator of the CSE query.

April 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	91	91	0	4	0.5 hrs
ARCHER2_CSE_Level2	74	71	32	13	0.3 hrs
ARCHER2_CSE_Level3	1	5	5	49	0.3 hrs
ARCHER2_CSE_TA	31	28	6	13	0.5 hrs
May 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	84	76	8	4	0.3 hrs
ARCHER2_CSE_Level2	77	80	29	15	0.2 hrs
ARCHER2_CSE_Level3	1	5	1	39	0.7 hrs
ARCHER2_CSE_TA	11	12	5	14	0.3 hrs
June 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	169	177	0	4	0.3 hrs
ARCHER2_CSE_Level2	66	69	26	13	0.3 hrs
ARCHER2_CSE_Level3	1	0	2	0	-
ARCHER2_CSE_TA	4	8	1	11	0.8 hrs
Q2 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	344	344	0	4	0.4 hrs
ARCHER2_CSE_Level2	217	220	26	14	0.3 hrs
ARCHER2_CSE_Level3	3	10	2	44	0.5 hrs
ARCHER2_CSE_TA	46	48	1	13	0.5 hrs

CSE Query Categories

A total of 622 queries were resolved by the ARCHER2 CSE service in the Reporting Period. Resolved CSE queries in the Reporting Period fell into the following categories:

Service level	Category	Number resolved	% Queries
ARCHER2_CSE_Level1	Courses	344	55.3%
ARCHER2_CSE_Level2	3rd Party Software	89	14.3%
	Batch system and queues	42	6.8%
	Compilers and system software	30	4.8%
	eCSE Applications/Calls	20	3.2%
	Login, passwords and ssh	11	1.8%
	User programs	7	1.1%
	Disk, tapes, resources	5	0.8%
	Data Transfer	4	0.6%
	Porting	4	0.6%
	Access to HPC	3	0.5%
	Performance and scaling	2	0.3%
	Courses	2	0.3%
	Other	1	0.2%
ARCHER2_CSE_Level3	Compilers and system software	5	0.8%
	3rd Party Software	3	0.5%
	Porting	1	0.2%
	Performance and scaling	1	0.2%
ARCHER2_CSE_TA	UKRI Grant	22	3.5%
	Access to HPC	12	1.9%
	Top up	6	1.0%
	Director Time	4	0.6%
	Pump priming	3	0.5%
	Non-UKRI Grant	1	0.2%
Total		622	100%

7. ARCHER2 Training

As part of ARCHER2, the service has been developing and delivering online an training programme for the ARCHER2 community. During the second quarter of 2021, the CSE service has provided a total of 12.5 days of online training, scheduled as follows:

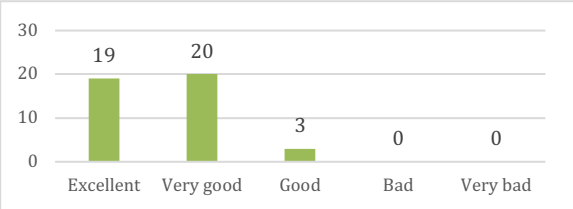
Dates	Course	Days	Attend
7 Apr 2021	Python on ARCHER2 for software package users	0.5	42
19 Apr 2021	Understanding Package Performance	1	3
20-22 Apr 2021	Efficient use of the HPE Cray EX Supercomputer ARCHER2	3	26
22-23 Apr 2021	QM/MM simulation with GROMACS + CP2K	2	28
2-3 Jun 2021	HPC Carpentry	2	13
14-17 Jun 2021	Data Carpentry	2	11
21-24 Jun 2021	Software Carpentry	2	22

Courses were not delivered in May as it was planned that the ARCHER2 machine would not be available during that period.

A new online self-service course on MPI was published in April. Self-service courses allow people to access training when it suits them, and registrations are always open. More than 100 people have already registered.

The ARCHER2 training panel meeting took place in early April. The results of the first year of the ARCHER2 training service were positively evaluated. The programme of courses for May 2021 – April 2022 was approved, and it is available on the training section of the ARCHER2 website.

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 4.4, i.e., better than "Very Good". Users provided 42 responses, a response rate of 41%.



The last run of the Software Carpentry course received a Net Promoter Score (NPS) of 50, according to The Carpentries pre- and post-workshop survey results. NPS vary between -100 and +100. A positive NPS is deemed good, a NPS of 50 or above is deemed excellent, and a NPS of 70 or above is exceptional. You can find more information about the NPS on Wikipedia.

8. ARCHER2 Embedded CSE Programme (eCSE)

As part of ARCHER2, the CSE service will deliver an eCSE programme to provide embedded CSE support across the UK. The service will deliver an average of 12 FTEs over its lifetime. Over the first 4 years of the ARCHER2 service this will provide 576 PMs.

eCSE Calls 1-4

- During the initial 4-year period of the contract, there are at least 576 PMs available under eCSE over some 8 calls, i.e., 72 PMs per call.
- Over the first 4 calls, 318 PMs have been awarded across 35 projects (as detailed in the table below), an average of 79 PMs per call.
- From the second call onwards, projects have been awarded to develop software from the NERC remit as well as from EPSRC. Projects from the NERC remit receive 10.73% of the awarded PMs, giving 514 PMs for projects within the EPSRC remit and 62 PMs for projects within the NERC remit.
- All of the 62 NERC PMs have now been allocated meaning from the fifth call onwards calls will be open to projects within the EPSRC remit only.
- The following table gives details of the proposals received and the projects awarded across the first 4 calls. To date, 63 proposals have been received requesting a total of 478 PMs with 35 projects having been awarded a total of 318 PMs.
- Some proposals fell within both EPSRC and NERC remits and were assigned a split (e.g. 80:20 EPSRC:NERC) which was agreed between the two research councils. When counting proposals or projects these have been counted according to which remit assigned the largest fraction, with the individual PMs then counted according to the agreed ratio.
- One project from the eCSE01 call is starting considerably later than planned (July 2021) having been delayed due to a previous project being extended for COVID-19 reasons.

eCSE call	Call open date	Tech eval deadline	# Tech evals rec'd	Final call deadline	# Props rec'd (EPSRC, NERC)	# PM req'ed (EPSRC, NERC)	#Props accep'd (EPSRC, NERC)	# PM Awardd(EPSRC, NERC)	# Projs started (EPSRC, NERC)	# Projs ended (EPSRC, NERC)
eCSE 01	19/05/20	16/06/20	25	07/07/20	25 (25,0)	235 (235,0)	13 (13,0)	132 (132,0)	12 (12,0)	0 (0,0)
eCSE 02	08/09/20	06/10/20	13	27/10/20	12 (9,3)	107 (87,20)	7 (4,3)	53 (33,20)	7 (4,3)	0 (0,0)
eCSE 03	08/12/20	23/02/21	15	16/03/21	14 (10,4)	136 (105,31)	8 (6,2)	73 (54,19)	3(2,1)	0 (0,0)
eCSE 04	20/04/21	18/05/21	13	08/06/21	12 (9,3)	109 (83,26)	7 (4,3)	60 (37,23)	0 (0,0)	0 (0,0)
Total			66		63 (53,10)	587 (510,77)	35 (27,8)	318 (256,62)	22 (18,4)	0 (0,0)

Future eCSE Calls

Calls will be issued three times per year with a regular timetable based on similar dates to those for the calls described above. The 5th ARCHER2 eCSE call (ARCHER2 eCSE05) opens on the 7 Sep 2021 with the deadline for submitting documents for technical evaluations on 05 Oct 2021 and the final deadline for proposal submission being 16:00 on 26 Oct 2021. An early career observers call will run alongside this call.

9. ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Community Engagement and Impact

The ARCHER2 team have been publicising the service, technical developments and the science being run on it in a series of blog articles. This quarter, 8 blog articles have been published and are available on the ARCHER2 website https://www.archer2.ac.uk/about/news/blog. Highlights have included a user article describing urgent modelling done of the active volcano in Fagradalsfjall, Iceland, looking at the spread of volcanic gas produced with its impact on health. The research software available to users on ARCHER2 was the subject of another post, and there was an interesting post from UKRI describing their role in the delivering and managing the ARCHER2 service. Two case studies are under development, one giving further details on the volcanic eruption research, and one on research run on ARCHER on amorphous silicon under high pressures which was featured on the cover of Nature Magazine in January 2021 https://www.nature.com/nature/volumes/589/issues/7840.

Outreach Activities and Events

- Planning for the International HPC Summer School (IHPCSS) is in the final stages – the event will be held virtually in the last two weeks of July, with every session happening twice to accommodate participants in different time zones (USA, Canada, Europe and Japan). The organisers are applying various tactics to ensure the all-online format still creates an inclusive, interactive and engaging opportunity for students to learn more about HPC, and to interact with their peers and mentors. CSE staff members are involved in teaching one of the tracks, running the mentoring programme, organising the programming challenge, and creating the virtual instance for the social and mentoring activities.
- Weronika Filinger (CSE team) is involved in running two ISC'21 sessions dedicated to online HPC education and training. The first one is a Birds of a Feather session on *Scalable and Effective online HPC education and training*. The second one is a session held during the third workshop on HPC Education and Training for Emerging Technologies. This session is titled *Hands-on, interactive exploration of tools to encourage and facilitate engagement*. The HPC community should embrace the opportunities associated with online learning platforms and methodologies. The benefits are not limited to scalability; they also include increased accessibility and inclusivity, compared to in-person alternatives.
- Weronika Filinger, as the chair of Student Programming, is also responsible for organising the student program during the SC21 conference. To reach as many students across the globe as possible, most of the sessions will be virtual and free of charge for the student attendees. The program will include sessions focusing on career progression, technical skills, as well as non-technical skills that are required for people to thrive in an HPC-related career. One of the goals is to feature different HPC job types, along with the people doing them all over the world, and information on how to get an HPC-related job. A number of workshops and drop-in sessions aiming to improve CV writing and elevator pitch are also planned.
- Women in HPC welcomed two new regional chapters during the period, including a successful application for Chapter status from the UK's N8 consortium of universities. This brings the number of UK-based WHPC Chapters to four (out of 17) with EPCC, the Numerical Algorithms Group, and the Thomas Young Centre running the other three.
- The ARCHER2 service was represented on EPCC's virtual booth at ISC'21, with the video of the build of the ARCHER2 system being shown.
- The ARCHER2 service has been accepted for the UoE's Images of Innovation Exhibition at the UN Climate Change Conference (COP26). In addition to an image of the service, there is information on the service and it's approach to equality, diversity and inclusion.

- Lorna Smith presented at the AMD HPC User Forum, associated with ISC'21. The forum provides opportunities to share best practice with interesting discussion points around singularity and package installation software such as Spack and Easybuild.
- A donation of £1 per user feedback response has been made to our selected charity, Save the Children. This quarter a total donation of £253 has been made, with £130 from the CSE Query feedback.

Quality Management and Information Security

EPCC puts the greatest importance on delivering the ARCHER2 service to best meet the needs of its users and the Research Councils, and to meet and exceed all contracted metrics. To ensure that we do this consistently, we have developed an ISO 9001 quality management system, which provides a framework for us to consistently review the service, the feedback provided by users and the Research Councils and service metrics and to identify areas for improvement. These improvements are then tracked to ensure that they deliver the benefits intended. We run a programme of internal audits throughout the year and have an annual external audit to ensure that we are meeting the requirements of the standard. We have been taking this approach for 5 years now, and whilst it does add additional workload, it has proved very effective and has become embedded as the way we work.

With the increasing importance of data in research, and the risks from cyber crime, in 2018 EPCC decided to add ISO 27001 certification for the services we run, including ARCHER2. We have developed an Information Security Management system and use this to ensure we meet the threat landscape and risk appetite of our users as regards information security. We have grouped the user data held into 4 categories, ranging from public data that might be available on a public website, through to restricted data that might include medical data. Each of these categories have security rules attached to it which we comply with. We run a programme of internal audits throughout the year, and have an annual external audit to ensure that we are meeting the requirements of the standard and applying best practice.