ARCHER2 CSE Quarterly Report

October– December 2024

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ARCHER 2 CSE Quarterly Report

This report covers the period October 2024 – December 2024 for the ARCHER2 service.

ARCHER2 Executive Summary

- The CSE team is working closely with HPE and the SP team to understand the potential options for a significant software upgrade to ARCHER2, looking to ensure any upgrade delivers value and minimises disruption to users.
- The second GPU call received 69 proposals requesting a total of around 1350 person months. At the panel meeting on 2/12/2024 proposals were ranked and 4 proposals were funded. Many of the proposals were of very high quality and the call was very competitive.
- A total of 18 days of training have been delivered as part of the ARCHER2 CSE training programme. Technology companies, such as AMD and Codeplay, have collaborated with us to deliver training to exploit the capabilities of GPUs.
- The CSE team has launched a suite of tools to help ARCHER2 users estimate the environmental impact of their computing simulations and workloads. The tools allow users to compare the greenhouse gas emissions associated with their use of the service to other common sources of emissions to try to help users understand how emissions from ARCHER2 compare to other activities.
- The ARCHER2 CSE service was well-represented at both Supercomputing 2024 and Computing Insight UK 2024. CSE staff were also key to delivering an ambitious and successful Women in HPC programme at SC24.
- The ARCHER2 Image competition was successful, with a wide range of high quality science on show. One of the entries appeared on advertising boards at SC24 as part of Art of the HPC, showcasing UK science on an international stage.
- The CSE team is currently involved in relocating centrally supported software to a less contended work filesystem to improve responsiveness and availability in light of contention issues on ARCHER2 work filesystem #1.
- The Spack Package Management System has been previewed to early adopters and is now available on ARCHER2 for users along with supporting documentation. In parallel, we have expanded the Reframe test suite to accommodate additional validation required for Spack-based software management.
- The outreach team travelled to New Scientist Live at the ExCel in London to showcase the service. The three-day event had over 25,000 visitors and provided a good opportunity to highlight the societal and economic value of supercomputing.
- As part of our work experience programme, we hosted 5 school-age students for a week of work experience In October 2024, providing opportunities for students interested in learning about post-education career possibilities in STEM.

ARCHER2 Forward Look

- The CSE team will continue to work closely with HPE and SP to understand the best options for a potential significant software upgrade to ARCHER2.
- During this next period, the CSE team will progress a plan for a Spack environment of centrally supported software and look to roll out Spack Package Management to a wider user base.
- HPE is expecting to complete the deployment of PowerSched on the ARCHER2 TDS by the end of January. This is a tool for dynamically adjusting the CPU frequency of compute nodes during running jobs to realise energy efficiency improvement. Once PowerSched is deployed, the CSE team will carry out an evaluation of the tool.
- Following a successful event last year, the ARCHER2 Celebration of Science will be run on the 14th and 15th May with the aim of showcasing ARCHER2 science and bringing together the ARCHER2 community. The CSE team will be developing the programme and preparing for this event during this period.
- The eCSE team will continue to support the range of eCSE projects currently underway and ensure scientific highlights are made available on completion of successful projects. We plan to promote the outputs of the eCSE programme at the Celebration of Science.
- A wide range of courses will be delivered in early 2025. Among them, the HPE Centre of Excellence will deliver a three-day course on leveraging the use of ARCHER2, including the AMD GPU Development platform.
- The outreach team will be preparing for the Edinburgh Science Festival in April, with a stand at Dynamic Earth for 5 days. The event will be open to the general public and we will have interactive exhibits highlighting the value of supercomputing and the benefit of careers in STEM.

ARCHER2 Centralised CSE Team

CSE has been active on various fronts over the period, helping to improve the ARCHER2 service, engaging with the community, and raising the profile of UK HPC internationally.

One highlight has been the rollout of new tooling to help people estimate emissions associated with their use of ARCHER2. Led by Andy Turner, the CSE team has launched a suite of tools to help users and prospective users of the service estimate the greenhouse gas emissions associated with their actual use of the service or their proposed use of the service. The methodology for estimating emissions and a full description of the tools can be found in the ARCHER2 documentation.

As well as estimating the emissions associated with historic use of ARCHER2, the tools allow users to compare the emissions to other common sources of emissions; to try to help users understand how emissions from ARCHER2 compare to other activities.

Following on from recent intermittent issues with ARCHER2 work file-system performance, the CSE team is working to relocate centrally supported software from its current location on work filesystem #1 (which is the most contended file system) to the generally quieter work filesystem #4. At the time of writing, the bulk of the work is complete and the *switch-over* is due to happen in the week beginning 13th January.

Two significant conferences featured in the calendar in the final quarter of 2024. During 17th—22nd November, the Supercomputing 2024 conference was held in Atlanta, USA, with various ARCHER2-related contributions from EPCC staff, including ARCHER2 publicity on the EPCC booth, contributions to the Women in HPC programme and other EDI sessions (described later), various outreach activities (also described later) and a CUG Xtreme meeting (special interest group for centres hosting large Cray supercomputers, for which Juan Rodriguez Herrera is an Executive Board member).

James Richings represented ARCHER2 at various SC24 events, including a meeting with key HPE staff (and representatives from ARCHER2 SP) to review progress with the ARCHER2 software upgrade project. James also participated in an Nvidia user-group meeting plus gathered information on key HPC technology news via vendor briefings and the technical programme.

Then during 5th—6th December, CSE participated in the Computing Insight UK meeting in Manchester, including hosting an ARCHER2 booth (also showcasing Cirrus Tier 2). James Richings also contributed to a Reframe training course, in collaboration with Tuomas Koskela (UCL), for which ARCHER2 was the training platform.

Juan Rodríguez Herrera (EPCC) contributed a talk to a new initiative that emerged from RSECon 2024, called “Charlas RSE en español”. Started by Carlos Gavidia-Calderon of the Alan Turing Institute and Sofian Minano from the Sainsbury Wellcome Institute at UCL, the initiative aims to showcase research software engineering to the Spanish-speaking international community (for example, in Europe and the Americas). Juan gave the first talk for the initiative, on 18th November, entitled "Aventuras y desventuras de ARCHER2, el servicio de supercomputación del Reino Unido".

Building on previously reported work on HPC-based Quantum Computing applications and simulations, Michael Bareford gave a presentation entitled “*The Scalability of Quantum Air Traffic Control*”, on 20th November, to the Quantum Computing Applications Cluster at Strathclyde University.

Michael Bareford had an opportunity to showcase this work to the Minster of State for Science, Research and Innovation, Lord Patrick Vallance, during a recent visit by the minister to the University of Edinburgh Informatics Forum. Michael explained the work we have done using ARCHER2 as a quantum-computer simulator and how this work is an enabler for research in quantum computing.

Continual Service Improvement (CSI) Projects

Likwid Performance Profiling

The work to add the Likwid performance-monitoring toolkit to ARCHER2, started in the previous period, is close to completion. Some issues were identified regarding the precision of one of Likwid's metrics, which CSE team member, Arno Proeme, has worked to address. Arno's improvements have been passed back to the Likwid developers for inclusion in the main code base. Likwid will be officially released to the user community in the near future.

PowerSched Evaluation

PowerSched is a tool for dynamically adjusting the CPU frequency of compute nodes during running jobs, intended to realise energy efficiency improvements. The tool has been developed by HPE and staff at the HLRS supercomputing centre (Germany), where it has been in use for a year or so. Following on from a presentation by the PowerSched team in Summer 2024, the CSE team has kicked off an evaluation, as noted in the previous report, initially installing and validating Likwid (a profiling tool on which PowerSched depends).

During this period, the HLRS team – working with local HPE staff in Edinburgh – has determined how to set up PowerSched on an HPE CSM-based system like ARCHER2 (HLRS use a different management software, called HPCM) and, at the time of writing, is installing PowerSched onto the ARCHER2 TDS system. In parallel, CSE defined a testing strategy for the software and recorded baseline performance measurements on TDS.

HPE is expecting to complete the ARCHER2 TDS PowerSched deployment by the end of January, at which point the CSE evaluation can progress further.

Spack Package Management on ARCHER2

A version of Spack is now available on ARCHER2 for end-users along with supporting documentation, presented as a technology preview. That is, we have invited power users to experiment with or use the software but have not yet formalised a recommendation for how the wider user community could exploit Spack.

During the period, the CSE team (specifically, Luca Parisi, Eleanor Broadway, and Rui Apostoli) have continued to grow its understanding of Spack, including formulating an approach to in-place upgrading the software and progressing a plan for a Spack *environment* of centrally supported software. The intention is to default to using Spack for centrally supported software packages, except where it is not suitable (for example, there is no suitable Spack configuration for software, or the Spack configuration produces a sub-optimal version of the package).

Reframe-Spack Integration

Running in parallel with the work on Spack Package Management, noted above, Eleanor Broadway, James Richings, and Juan Rodriguez Herrera have expanded the Reframe test suite to accommodate additional validation required for Spack-based software management.

As noted above, the previously reported work to develop good practice for use of Reframe on HPC was presented in a workshop at Computing Insight UK.

ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from October 2024 – December 2024.

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. *MTR applicable to OY5: Service Threshold: >4 WD; Operating Service Level: >1 WD, ≤2 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. *MTR applicable to OY5: Service Threshold: >25 Working Days (WD); Operating Service Level: >10 WD, ≤15 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. *MTR applicable to OY5: Service Threshold: >55 Working Days (WD); Operating Service Level: >25 WD, ≤35 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 OY5: 6 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	Oct 2024		Nov 2024		Dec 2024		Q4 2024	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	0.1WD	-2	0.1WD	-2	0.1WD	-2	0.1WD	-6
ARCHER2_CSE_Level2 (MTR)	0.2WD	-2	0.3WD	-2	0.6WD	-2	0.4WD	-6
ARCHER2_CSE_Level3 (MTR)	-		31WD	0	-		31WD	0
ARCHER2_CSE_TA (%)	100%	-1	100%	-1	100%	-1	100%	-3
Initial Response to Queries (%)	100%	-1	99.4%	-0.25	98.8%	0	99.6%	-1.25
Query User Satisfaction (%)	100%	-2	100%	-2	100%	-2	100%	-6
Training Satisfaction (%)	100%	-1	100%	-1	100%	-1	100%	-3
Total		-9		-8.25		-8		-25.25

73 query feedback responses were received on query resolution in the Reporting Period. 100% of responses had a score of “Good”, “Very Good” or “Excellent”.

ARCHER2 CSE Queries

This section provides details on ARCHER2 CSE queries during the Reporting Periods from October 2024 – December 2024.

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.

Oct 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	218	217	3	3	0.3h
ARCHER2_CSE_Level2	64	59	22	12	0.3h
ARCHER2_CSE_Level3	0	0	1	0	-
ARCHER2_CSE_TA	4	3	2	6	0.2h
Nov 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	90	93	0	3	0.3h
ARCHER2_CSE_Level2	55	48	29	12	0.3h
ARCHER2_CSE_Level3	0	1	0	11	0.3h
ARCHER2_CSE_TA	12	13	1	10	0.4h
Dec 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	23	23	0	3	0.5h
ARCHER2_CSE_Level2	44	52	21	13	0.3h
ARCHER2_CSE_Level3	1	0	1	0	-
ARCHER2_CSE_TA	8	9	0	8	0.6h
Q4 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	331	333	0	3	0.3h
ARCHER2_CSE_Level2	163	159	21	12	0.3h
ARCHER2_CSE_Level3	1	1	1	11	0.3h
ARCHER2_CSE_TA	24	25	0	9	0.4h

CSE Query Categories

A total of 518 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	333	64.3%
ARCHER2_CSE_Level2	3rd party software	33	6.4%
	Software installation	19	3.7%
	Batch system and queues	17	3.3%
	Compilers and system software	13	2.5%
	Software errors	13	2.5%
	Courses	12	2.3%
	eCSE applications/calls	11	2.1%
	Login, passwords and ssh	10	1.9%
	Porting, performance and scaling	10	1.9%
	Data transfer	7	1.4%
	User behaviour: Queries relating to user behaviour	4	0.8%
	Access to services	3	0.6%
	Other: Queries which do not fit within other categories	3	0.6%
	Hardware issue	2	0.4%
	SAFE: Queries relating to SAFE	1	0.2%
	Storage and compute resources	1	0.2%
ARCHER2_CSE_Level3	3rd party software	1	0.2%
ARCHER2_CSE_TA	Grant	13	2.5%
	Pump-priming	7	1.4%
	Director's Time	4	0.8%
	Access to HPC	1	0.2%
Total		518	100.0%

ARCHER2 Training

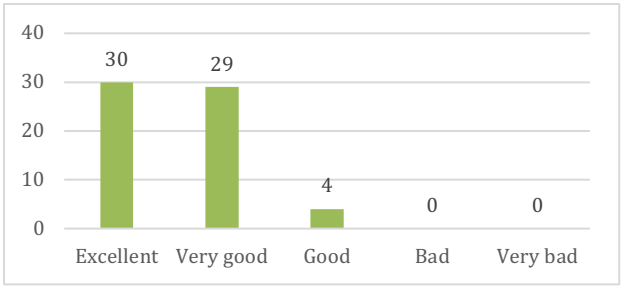
As part of ARCHER2, the service has been developing and delivering a training programme for the ARCHER2 community. During the last quarter of 2024, the CSE service has provided a total of 18 days of training, scheduled as follows:

Dates	Course	Location	Days	Attend
1-4 Oct	Accelerating your Applications with AMD GPUs	Online	2	40
15 Oct	Efficient Parallel IO	Online	1	12
17 Oct	Introduction to LAMMPS	Online	1	19
21-22 Oct	Data Analysis and Visualisation in Python	Online	2	17
24 Oct	Exploring new computational frontiers with SmartSim	Online	0.5	22
12-13 Nov	Single Node Performance Optimisation	Edinburgh	2	12
18-19 Nov	HPC Carpentry	Newcastle	2	20
26-27 Nov	Message Passing programming with MPI	Birmingham	2.5	18
26-28 Nov	Intermediate Research Software Development	Belfast	3	31
2, 9 Dec	Introduction to LAMMPS	Online	1	14
3 Dec	Cross-vendor GPU development with C++ and SYCL	Online	1	11

Leading technology companies, including AMD and Codeplay, have collaborated with us to provide training courses designed to exploit the advanced capabilities of GPUs. Also, we added an additional run of the LAMMPS course due to high demand.

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 63 responses, a response rate of 32%.



ARCHER2 and GPU Embedded CSE Programme (eCSE)

ARCHER2 eCSE Programme

The ARCHER2 eCSE programme awarded 806 PMs across 11 calls, exceeding the contractual requirement of 798 PMs. No further ARCHER2 eCSE calls will be opened in the near future.

GPU eCSE

- The 4 projects funded from the second call will start within the first half of 2025. One of the 4 projects was partially funded from remaining ARCHER2 funds.
- Across the 2 calls, 12 projects have been awarded a total of 319 person months.
- The initial allocation of funds for the GPU calls has now been awarded in full. The opening of any future calls will be dependent on receiving further allocations of funding.

	1st GPU call				2nd GPU call			
Research Councils	# Props	# PMs	# Props award	# PMs award	# Props	# PMs	# Props award	# PMs award
ESRC (Economic and Social Research Council)	3	55	0	0	3	58	0	0
EPSRC (Engineering and Physical Sciences Research Council)	31	749	6	186	45	877	2	39
STFC (Science and Technology Facilities Council)	12	279	2	456	12	262	1	24
NERC (Natural Environment Research Council)	4	88	0	0.0	9	155	1	24
MRC (Medical Research Council)	1	12	0	0.0	0	0	0	0
Total	51	1183	8	232	69	1352	4	87
Total (both calls)					120	2535	12	319

ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Benefits Realisation

Three case studies have been published this quarter, highlighting the important science being carried out on ARCHER2 and the impact of the computational science provision. The case studies spanning different areas of science were:

- High fidelity simulations to improve performance and safety of nuclear reactors
- Solvation and charge transfer processes at semiconductor/liquid water interfaces
- Simulating a flexible infectious viral protein

Blogs

Eleven blogs have been published this quarter. Highlights included the work done on the estimation of emissions from ARCHER2 and the jobs run on it. Another blog was written giving background and details about one of our ARCHER2 Early Career researchers, timed to coincide with the publication of their Pioneer project case study on an infectious viral protein. The launch of the GPU Driving Test was highlighted plus work on visualisations of wind turbine flow and the use of GeoChemFoam for pore-scale modelling.

Community and Outreach Activities

The Supercomputing 2024 conference provided several good opportunities for the ARCHER2 team. Eleanor Broadway organised an HPC Scavenger Hunt that ran throughout the conference, designed to showcase some of the amazing outreach activities which the HPC community already engages in, hoping to inspire others to get creative and join in. The hunt was a collaboration between EPCC, the Texas Advanced Computing Center, the US Department of Energy, IT4Innovations National Supercomputing Center and Georgia Institute of Technology. The prize draw was conducted at the EPCC booth, drawing a crowd of around 30 people.

Eleanor also led the organisation of a SC24 Birds of a Feather session on "HPC Outreach: Mastering the Art of Science Communication". The session invited the community to share experiences and gather strategies around science communication, on how to engage with different audiences and change the delivery/language/focus of your topic.

Also at Supercomputing, Weronika Filinger contributed two talks to the 11th SC Workshop on Best Practices for HPC Training and Education.

The outreach team travelled to New Scientist Live at the ExCel in London to showcase the service. The three-day event had over 25,000 visitors and provided a good opportunity for us to exhibit outside our local area and to talk about how EPCC and ARCHER2, the UK national supercomputing resource, support important scientific research. With one day dedicated to schools groups, this was also a great opportunity to both educate and promote STEM careers to young people.

In October 2024, EPCC hosted 5 school-age students for a week of work experience. These students were interested in learning about post-education career possibilities in STEM. Through an ACF tour, talks from staff members, and completion of a mini project they gained insight into what it might be like to work here. This also allowed us to trial a new standard offering for a week of work experience, which we aim to repeat twice annually.

Diversity and Inclusivity

Supercomputing is the biggest event on the annual Women in HPC calendar and, as always, the ARCHER2 team was heavily involved in the planning, organisation and delivery of the programme, which included:

- A WHPC Workshop titled: "Building Community", at which Eleanor Broadway was the Fellowships and Submissions Chair.
- Ran a session on WHPC Chapters and Affiliates, introducing the SC24 community to the WHPC Chapters and Affiliates, discussing their purpose, mission, latest updates and how to get involved.
- Organised the annual Chapters and Affiliates meet-up, which brought together members of the WHPC Chapters and Affiliates meet-up to network. Around fifteen chapters and affiliates were represented.
- Following its reinstatement in 2024, the WHPC Mentor Programme continued at SC, with James Richings contributing as a mentor for early career researchers.

Quality Management, Information Security and Business Continuity

The annual work to ensure we are applying and improving our policies, processes and technical controls continues, ensuring that we deliver the best possible level of service to our users, keeping their data safe and maximising the uptime and availability of all the services we run. This is done by a program of internal audits, regular reporting on performance and monitoring of external resources to ensure we apply best practice.