ARCHER2 Quarterly Report

July– September 2024

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ARCHER 2 Quarterly Report

This section of the report covers the period July 2024 – September 2024 for the ARCHER2 service.

ARCHER2 Executive Summary

- CSE completed a refresh of the Centrally Supported Software on ARCHER2, carried out periodically to track community requirements and realise trends in scientific computing. The PyTorch machine-learning framework, Blender visualisation package, and the Likwid tool have all been added.

- Installation of the Likwid performance analysis tool is a prerequisite for the PowerSched power/performance tool that has been deployed on a peer system in HLRS, Germany, with consequent improvements in energy efficiency. The CSE team is currently working on developing good-practice and training material to support its use.

- CSE were highly visible at RSECon ’23, running a booth, contributing to the workshop programme and presenting a talk on the “Environmental sustainability of ARCHER2”.

- CSE assisted with the Capability Days #3 activity, 24th—26th September, running a “how-to” webinar which included good practice on file system use and package management, based on our findings from the previous two Capability Days sessions.

- A further expansion of Reframe has been undertaken, to include more performance monitoring. This is useful to checking changes to the ARCHER2 system environment and software do not degrade performance.

- The team is working with colleagues from HPE on the Software Upgrade working group, which is investigating options for maintaining the security and functionality of the HPE software that runs ARCHER2 while minimising the need for significant outages.

- The second GPU eCSE call received a significant number of proposals, demonstrating the need for funding of this type within the community. Funding decisions are expected to be made after the panel meeting which is planned to take place in late November.

- The outreach team attended the Biggar Science Festival on the 13th September in Biggar, South Lanarkshire, with good engagement from local attendees.

ARCHER2 Forward Look

- The Outreach team is attending New Scientist Live in London in October, hosting a booth for the 3-day event and highlighting the value of Supercomputing to the General public.

- Women in HPC has prepared its most ambitious programme, to date, for Supercomputing 2024, including the Women in HPC workshop on diversity and inclusivity, the biggest SC'24 Diversity Day to date, the WHPC Networking Reception, and the WHPC mentor programme.

- Several training projects focused on leveraging the use of accelerators are currently in development, promising to enhance the computational skills of the ARCHER2 user community.

- The team will be looking to analyse usage patterns and outcomes from the recent Capability Days, to help plan for future Capability Days, minimising disruption while maximising value.

- The service improvement team will continue to develop good-practice notes and material for a webinar on Likwid, to help people gain experience of this tool.

- The team will continue to expand the pool of Spack packages in the next period, plus are investigating whether Spack provides a tangible way to support Python Modelling Frameworks, which are otherwise very difficult to support in a shared environment.

- The second GPU eCSE panel meeting will take place during this quarter, awarding a second round of funding to successful projects.

ARCHER2 Centralised CSE Team

This has been a busy and productive period for the CSE team, with a mix of service-improvement activities, outreach and user engagement, plus continuing to develop the ARCHER2 service.

In the previous reporting period, we initiated a review and refresh of the centrally supported software on the service. This is something CSE do, typically, annually to track community requirements and realise trends in scientific computing. The refresh completed during July—August, with details in Request for Change AR2-RFC-0202. Highlights include the addition of the PyTorch machine-learning framework, Blender visualisation package, and the Likwid profiling tool. Complementing this. we rationalised the scientific-libraries list, removing several packages that are no longer well-used in the community.

Likwid is also the subject of a Service Improvement activity, which is described below. Likwid is a prerequisite for the PowerSched power/performance tool that has been deployed on a peer system in HLRS, Germany, with consequent improvements in energy efficiency.

The, now annual, RSECon conference returned to Newcastle, during 3rd—4th September. CSE was well-represented: helping to run an ARCHER2; leading an HPC RSE session; and contributing four sessions for the main programme:

- Adrian Jackson, Alan Simpson, Lorna Smith, Andy Turner, *Environmental sustainability of ARCHER2*
- Andy Turner et al. HPC RSE Birds of a Feather – in collaboration with RSEs in Cambridge, Imperial College and UCL
- Juan Rodriguez Hererra participated in the panel for the *RSECon2024 Community Discovery Day Birds of a Feather*
- Kirsty Pringle, Andy Turner, et al. *Green RSEs? Building a community to reduce the environmental impacts of research software (Birds of a Feather)* – in collaboration with BAS, Cambridge, NOC.
- Juan Rodriguez Hererra also co-chaired the RSE Training and Professional Development Birds of a Feather, from which a SIG proposal was submitted for review to The Society of Research Software Engineering.

The CSE team also began work, with colleagues from HPE, on the Software Upgrade working group, which is investigating options for maintaining the security and functionality of the HPE software that runs ARCHER2 without the need for significant outages. We will provide more information on the progress of the working group in the next reporting period.

Towards the end of the period, we helped run Capability Days #3 session, during 24th—26th September. CSE delivered an ARCHER2 webinar to promote the service, including good practice on file system use and package management, based on our findings from the previous two Capability Days sessions.

James Richings represented ARCHER2 on the EPCC stand at the Operational Research Society Annual Conference (Bangor University, 10th—12th September). There was a good level of interest in ARCHER2, with introductions made to around 20 potential new users.

Rui Apostolo (funded by the UKRI-funded MPIC project) helped organise and deliver a workshop on using the EPIC software, a relatively new application for particle-in-cell modelling for fluid dynamics. The workshop, which was based on work undertaken on ARCHER2, was delivered on 8th—9th July as part of the ICTP Summer School in Trieste, and on 30th of September at Leeds University.

There were a small number of staffing changes, during the period. Michael Bareford left the CSE team to work on HPC research projects, though still assists with some software support and HEC/ NERC Consortia engagement activities. Linnea Gilius joined the team from September, initially as part of the Service Improvement Team.

Looking forward, it is a little over a month until Supercomputing 2024 (Atlanta, 17th—22nd November). CSE will be well represented, including a full Women in HPC programme (described later) and various other programme contributions that we will report on in the next period. One novel contribution is from Sebastien Lemaire (working with Michèle Weiland, EPCC, and Andrew Mole (Imperial College)) who have a visualisation, entitled *Sunset on Wind Turbines*, accepted into the Art of HPC session. The visualisation was created on ARCHER2 using Xcompact3D and Paraview.

Continual Service Improvement (CSI) Projects

Likwid Performance Profiling

As part of the software refresh, noted above, the Likwid performance tool has been added to the Centrally Supported Software list. Likwid is a sophisticated tool, mostly of interest to power users, though it provides powerful insight into the performance and energy consumption of an application. To help people gain experience of Likwid, we are developing good-practice notes and material for a webinar to be completed in the next reporting period.

Likwid is also a key dependency for the PowerSched evaluation; requirements for PowerSched are factored into the Likwid deployment configuration.

Spack Package Management on ARCHER2

Building on the work undertaken in previous period, Spack testing has accelerated and we have now installed a small number of Centrally Supported Applications via Spack. Spack has been integrated with the module system, Lmod, so no user-visible changes are observed.

We will continue to expand the pool of Spack packages in the next period, plus are investigating whether Spack provides a tangible way to support Python Modelling Frameworks, which are otherwise very difficult to support in a shared environment.

Performance Monitoring with Reframe

A further expansion of Reframe has been undertaken, to include more performance monitoring. This is useful for checking changes to the ARCHER2 system environment and software do not degrade performance, and will be particularly useful for the Software Upgrade working group, when they begin testing candidate upgrade paths.

Open on Demand

Open on Demand is a tool for enabling web-based access to shared use systems such as ARCHER2. Over recent times, it has gained popularity in the HPC community and is now deployed for a number of the UKRI Tier-2 services. Open On Demand has the potential to streamline access to HPC resources for new users and to simplify the setup of training courses. It can also support alternative workflow paths and interactive environments such as Jupyter notebooks.

The CSE team has set up a demonstration Open on Demand instance for the Cirrus Tier-2 service, aimed at providing a sandbox in which CSE staff can explore use cases and workflows. Initial reaction to the demonstration has been positive and we are proceeding to move to a more production footing for Cirrus. Looking forward, there is potential to deploy Open on Demand on ARCHER2, though we note there are several technical hurdles that would need to be addressed to do this.

ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from July 2024 – September 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	Jul 2024		Aug 2024		Sep 2024		Q3 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)	0.8WD	-2	1WD	-2	0.9WD	-2	0.6WD	-6
ARCHER2_CSE_Level3 (MTR)	-		24WD	-0.5	-		24WD	-0.5
ARCHER2_CSE_TA (%)	100%	-1	95.00%	0	100%	-1	96.55%	-2
Initial Response to Queries (%)	100%	-1	97.67%	1	100%	-1	99.41%	-1
Query User Satisfaction (%)	100%	-2	96.00%	-2	100%	-2	98.61%	-6
Training Satisfaction (%)	100%	-1	100%	-1	100%	-1	100%	-3
Total		-9		-6.5		-9		-24.5

72 query feedback responses were received on query resolution in the Reporting Period. 98.6% of responses had a score of “Good”, “Very Good” or “Excellent”.

Due to the change in the overall Access to HPC call, we introduced a new process for technical assessments (TAs) to minimise the delay in getting new projects onto ARCHER2. This process also allows for improved gathering and analysis of statistics. However, there were a number of minor teething problems with introducing this: one TA missed the TA Target Completion Date and 3 initial responses to the TAs were sent beyond 3 hours in this reporting period. The tracking issues that led to this have now been resolved.

ARCHER2 CSE Queries

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

Jul 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	80	79	1	3	0.2h
ARCHER2_CSE_Level2	44	48	17	13	0.2h
ARCHER2_CSE_Level3	0	0	1	0	-
ARCHER2_CSE_TA	6	4	2	11	0.1h
Aug 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	67	67	1	3	0.5h
ARCHER2_CSE_Level2	43	41	19	14	0.4h
ARCHER2_CSE_Level3	0	1	0	51	0.5h
ARCHER2_CSE_TA	20	20	2	7	0.2h
Sep 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	176	175	2	3	0.5h
ARCHER2_CSE_Level2	69	70	18	12	0.2h
ARCHER2_CSE_Level3	2	0	2	0	-
ARCHER2_CSE_TA	4	5	1	13	1h
Q3 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	323	321	2	3	0.4h
ARCHER2_CSE_Level2	156	159	18	13	0.3h
ARCHER2_CSE_Level3	2	1	2	51	0.5h
ARCHER2_CSE_TA	30	29	1	9	0.5h

CSE Query Categories

A total of 510 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	321	62.9%
ARCHER2_CSE_Level2	eCSE applications/calls	36	7.1%
	3rd party software	32	6.3%
	Batch system and queues	17	3.3%
	Software errors	15	2.9%
	Software installation	13	2.5%
	Porting, performance and scaling	11	2.2%
	Access to services	9	1.8%
	Courses	5	1.0%
	Login, passwords and ssh	5	1.0%
	Compilers and system software	4	0.8%
	Data transfer	4	0.8%
	Storage and compute resources	3	0.6%
	Other: Queries which do not fit within other categories	2	0.4%
	SAFE: Queries relating to SAFE	2	0.4%
	User behaviour: Queries relating to user behaviour	1	0.2%
ARCHER2_CSE_Level3	Software errors	1	0.2%
ARCHER2_CSE_TA	Access to HPC	16	3.1%
	Grant	9	1.8%
	Pump-priming	3	0.6%
	Directors Time	1	0.2%
Total		510	100.0%

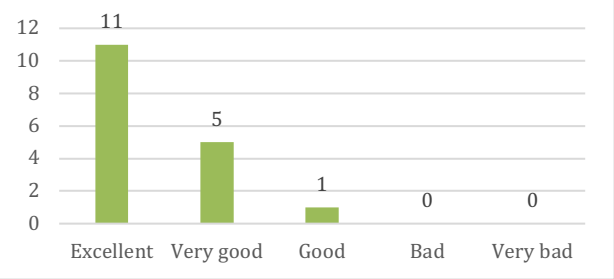
ARCHER2 Training

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

Dates	Course	Location	Days	Attend
7-9 Aug	GPU programming with HIP	Online	3	29
19-29 Aug	Shared memory programming with OpenMP	Online	2.5	20
21 Aug	Re-Introducing WHPC: How We're Driving Change […]	Online	0.5	17
18 Sep	ARCHER2 Capability Days	Online	0.5	8
25 Sep	Adventures and misadventures in hybrid programming	Online	0.5	31

A reduced number of training activities have been scheduled during the summer period, although more number and variety are expected for the next season/quarter.

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 4.6, i.e., better than "Very Good". Users provided 17 responses, a response rate of 35%.



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 8 projects funded from the first call have either started or will start within the next few weeks.

Research Councils	Number of proposals	Number of PMs	Number of proposals awarded	Number of PMs awarded
ESRC (Economic and Social Research Council)	3	55.0	0	0.0
EPSRC (Engineering and Physical Sciences Research Council)	31	749.2	6	186.0
STFC (Science and Technology Facilities Council)	12	278.6	2	45.8
NERC (Natural Environment Research Council)	4	88.0	0	0.0
MRC (Medical Research Council)	1	12.0	0	0.0
Total	**51**	**1182.8**	**8**	**231.8**

The second GPU eCSE call opened on 02/07/2024 and closed on 17/09/2024 for projects starting in the first half of 2025. The call received a significant number of proposals and the panel meeting is planned to take place in late November.

ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Blogs and Case Studies

Five blogs have been published this quarter. The majority are highlighting the science carried out by researchers who entered the image competition.

We continue to publish case studies on the ARCHER2 website providing a more in-depth look at the science being run on ARCHER2. We work with the researchers to ensure that the case studies are accessible to an interested but non-expert audience. This is a good opportunity for researchers, particularly early career researchers to publicise their science.

Community and Outreach Activities

During this quarter the outreach team attended the Biggar Science Festival on the 13th September in Biggar, South Lanarkshire. This is a relatively smaller science festival, with good engagement from local attendees. The team ran a "Power of Programming" workshop, where participants program micro:bit devices to help simulate virus spread and to learn about the concepts of programming.

The team has also been preparing for New Scientist Live in London during October, one of the larger events the team attends.

We have been successful in our application to the Edinburgh Science Festival - 14-18th April 2025. We will run a drop-in workshop at Dynamic Earth around the theme of "Spaceship Earth", highlighting the power of Supercomputing and also the importance of sustainability in the delivery of HPC services.

Four members of staff applied and were accepted to act as mentors in a Career Ready Mentoring Scheme. The scheme will run for ~18 months and involves mentoring local young people who face socio-economic barriers. This includes a 4-week placement at EPCC in June/July 2025.

Diversity and Inclusivity

Women in HPC has prepared its most ambitious programme, to date, for Supercomputing 2024 (https://womeninhpc.org/events/sc-2024), including the Women in HPC workshop on diversity and inclusivity, the biggest SC'24 Diversity Day to date, the WHPC Networking Reception, and the WHPC mentor programme. The WHPC Fellowship Programme has also sponsored two early-career researchers, from under-represented groups, to participate in the conference.

EPCC again contributed to the programme for the International HPC Summer School (https://ihpcss.org/). Specifically, Weronika Fillinger ran the mentoring programme and Ludovic Capelli taught on the GPU programming track and ran the programming challenge. Weronika is also a member of the organising committee and the mentoring committee.

Weronika Filinger has been working with the UNIVERSE-HPC project (https://www.universe-hpc.ac.uk/) to create more inclusive and accessible training ecosystem for RSEs. Weronika, working with several international collaborators – to help UNIVERSE-HPC develop guidelines to make the training content more FAIR – ran interactive surveys during Supercomputing 2023 from which the results have been reported in two PEARC'24 publications:

- Building HPC Learning Pathways: Understanding our community - https://doi.org/10.1145/3626203.3670513
- Developing HPC Learning Pathways: Challenges and Recommendations - https://doi.org/10.1145/3626203.3670575

Both publications are important steps towards improving professional development opportunities for Research Technical Professionals.

Quality Management, Information Security and Business Continuity

After the success of our ISO audits in June, we continue to work to identify improvements in the service we run, the information security measures we have in place and our business continuity plans. We are working towards our next major business continuity test. We identify particular aspects of the ARCHER2 service, or particularly topical risks and either run a full simulated exercise or a tabletop talk through how we would deal with the scenario. The last such exercise we ran looked at how a cyber security leak of data on to the internet would be handled. We are unable to say more about the upcoming test, but we always review lessons when we run a test to identify any improvements.