ARCHER2 Quarterly Report

April – June 2024

EPCC

The University of Edinburgh

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ARCHER 2 Quarterly Report

This section of the report covers the period April 2024 – June 2024 for the ARCHER2 service.

ARCHER2 Executive Summary

- The first GPU eCSE call closed on 19 March 2024 and received 51 proposals from 5 different research councils; 8 proposals were funded. The second call is now open. It is clear there is significant demand for the eCSE programme.

- An Early Career Observers call opened alongside the 1st GPU eCSE call. 11 applicants were accepted and will attend one of the eCSE GPU call panels.

- The CSE team arranged for a newer version of the Cray Programming Environment (Version 23.09) to be installed as a non-default version during this quarter. This should allow users to benefit from newer versions of the Cray and AMD compiler suites and improvements to the AMD ROCm environment (a key software library on the GPU Development System).

- As a result of feedback from the community, the team are developing a good-practice guide for users on how to write tests for the Reframe test suite. This should allow contributions from, and uptake within, the user community of the suite.

- The range of centrally installed software for the GPU Development System has been extended, adding the popular applications LAMMPS, GROMACS, and NAMD.

- We are now a member of Xtreme, a Special Interest Group within the Cray User Group organisation, focused on large-scale scientific/technical computing using HPE Cray systems.

- During this quarter we provided a total of 23 days of training including courses at Durham, York, Cambridge, London, Birmingham and Southampton.

- We attended the Big Bang Fair (19-21 June) at the NEC in Birmingham. Across the 3 days, over 20,000+ secondary aged children attended and our booth was busy for the full event.

- During this quarter we have supervised 5 students carrying out week-long work experience, offering them insight into the world of work.

- Women in HPC (WHPC) ran its most ambitious programme yet at ISC'24 (Hamburg, 12th—16th May) and were an official conference collaborative partner.

- EPCC recently passed our external audit for ISO 27001 (information security), ISO 9001 (quality service delivery) and ISO 22301 (business continuity).

ARCHER2 Forward Look

- A second GPU eCSE call opened in July and closes in September for projects running in the first half of 2025. This will finish the funding provided. It is clear that there is considerable demand for this type of funding and that many more high-quality proposals could have been funded had funding been available.

- The training plan for this year includes a GPU focus and additional training in this area is currently under development.

- The team plans to continue to develop the software available on the GPU system and support users to exploit this system. In particular, the team will work with the HEC BioSim consortium to evaluate key software on the GPU Development System.

- A significant number of students will carry out work experience at EPCC this summer, including 5 students from the Nuffield research programme who will visit us for 3 weeks.

- Planning is underway for New Scientist Live, which is at the ExCel in London in October, an event that introduces HPC to the wider public.

- EPCC has a booth at RSECon in September and we will use this to highlight ways for RSEs to access ARCHER2, through the eCSE and through calls for CPU time. The training programme will be highlighted as will opportunities to collaborate.

ARCHER2 Centralised CSE Team

This has been a busy, but productive, period for the CSE team with lots of opportunities to work with the ARCHER2 user community.

During the period, we participated in two, important international HPC conferences—the Cray User Group Meeting (Perth, Australia, 5th—9th May 2024) and ISC'24 (Hamburg, Germany, 12th—16th May). CSE was well-represented at both conferences.

At CUG, Juan Rodriguez Herrera (also current Director at Large, on the CUG Board of Directors) presented a paper from the CSE team -- "Scalability and Performance of OFI and UCX on ARCHER2" in the main programme and gave a talk entitled "EPCC's ReFrame testing strategies for ARCHER2 and Cirrus" on the "HPC System Testing Workshop", a satellite event that took place before the main meeting. Further, Adrian Jackson presented at the ExaDigiT digital twin BoF, discussing the work we are doing on ARCHER2 to model and optimise the system, including looking at the power and cooling systems that support the system. Adrian also presented a tutorial on new storage technologies, particularly focusing on object storage approaches and how they can be exploited by computational simulation applications.

Following on from CUG, EPCC is now a member of Xtreme, a Special Interest Group (SIG) within the CUG organisation, focused on large-scale scientific/technical computing using HPE Cray systems with particular emphasis on early deployment (beta or early production): Tools Development, Networking, I/O, Resource Management, System Administration, Service, Documentation, and Training.

For ISC, Andrew Turner was part of the organising committee for the RSE HPC workshop, which also featured two presentations from Eleanor Broadway on Fostering Early Career Skill Development in HPC and RSE: Leveraging Community Support. Eleanor, with Weronika Filinger, also presented a session called HPC Outreach: Telling our Stories at the HPC in Science BoF.

Closer to home, the CSE team also participated in the Durham HPC Days (16th—19th May). Andrew Turner (and, also from EPCC, Nick Brown) ran a session looking at the UK HPC Community and Eleanor Broadway contributed to a WHPC co-located event. Chris Rae (who has a work placement in EPCC) presented on his work to develop machine learning benchmarks and to incorporate them into the ARCHER2 Reframe suite.

Members of the CSE team also contributed to various domain-science events including:

- Rui Apostoli and Julien Sindt took part in the RSC "Molecular Simulations in Chemistry" event on Friday 14th June. EPCC hosted a stand there to promote ARCHER2 and engage with the researchers.
- Andy Turner participated in the Physical Sciences Data Infrastructure (PSDI) Town Hall meeting, on 20th June 2024, IMMM, London, UK

Chris Rae wrote a paper, based on his work placement, on how to speed up ML training by trading memory for reduced computation. This looked at multiple machines and the performance benefit across different ML models. This work helped members of the ARCHER2 team better understand the details on ML performance. The paper has been submitted to a conference and we await the outcome of this.

In June, EPCC hosted two visitors—Erik Draeger and Kristi Belcher—from Lawrence Livermore National Laboratories, who work on the US Exascale Compute Project. The focus was on the provision and operation of Exascale HPC services, as part of our work to get ready for the next generation of UK HPC services.

The User Advisory Group meeting was held on 14th May, with CSE being represented by Lorna Smith, Andrew Turner and George Beckett. The CSE team provided updates on the GPU Development System,

the Spack package management system, and addressed feedback and questions from other stakeholders and from the user community representatives.

Continual Service Improvement (CSI) Projects

Cray Programming Environment Update

In May, the CSE team arranged the installation of a newer version of the Cray Programming Environment (Version 23.09) to, amongst other things, allow users to benefit from newer versions of the Cray and AMD compiler suites and improvements to the AMD ROCm environment (a key software library on the GPU Development System).

CPE 23.09 was installed as a non-default version, allowing users to transition at their own pace, and providing continuity. It was also noted that CPE 23.09 is supported on newer versions of the Cray Operating System (whereas the previous version is not) meaning a smoother transition for users if an upgrade to the Operating System is actioned.

Spack Package Management on ARCHER2

Initial testing of a Spack Package Management environment on ARCHER2 by CSE (described in the previously quarterly report), highlighted some potential limitations and weaknesses. Further refinements have been made to address these limitations, including, coincidentally, improvements realised as part of the CSE 23.09 update. A second round of testing will be done by CSE during July and August and, all going well, we expect to invite some experienced users from the ARCHER2 community to evaluate the system before the end of the next quarter.

Reframe Test Suite Improvements

CSE's work to develop a Reframe test suite has attracted the attention of the HPC community – e.g., through CUG and Durham HPC Days presentations. Based on this feedback, we are developing a good-practice guide for how to write tests, which should allow contributions from and uptake within the user community of the suite.

Furthermore, we have integrated Reframe in the CheckMK monitoring system operated by SP to give live status information on the health of the ARCHER2 service. Going forward, this allows us to detect and respond more quickly to problems in the ARCHER2 programming environment and user interfaces, and allows us to more easily track trends in, for example, system performance.

GPU Supported Software

The CSE team has extended the range of centrally installed software for the GPU Development System, adding the popular applications LAMMPS, GROMACS, and NAMD. These additions will be publicised to the user community in July, allowing users to start to test the portability of their key simulations to a GPU platform.

ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from April 2024 – June 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	Apr 2024		May 2024		Jun 2024		Q2 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)	0.9WD	-2	0.2WD	-2	0.3WD	-2	0.6WD	-6
ARCHER2_CSE_Level3 (MTR)	-	-	14WD	-2	24WD	-0.5	23WD	-2.5
ARCHER2_CSE_TA (%)	100%	-1	100%	-1	100%	-1	100%	-3
Initial Response to Queries (%)	100%	-1	100%	-1	100%	-1	100%	-3
Query User Satisfaction (%)	100%	-2	100%	-2	100%	-2	100%	-6
Training Satisfaction (%)	98.25%	-1	100%	-1	100%	-1	98.72%	-3
Total		-9		-11		-9.5		-29.5

89 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 April 2024 – June 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.

Apr 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	152	158	0	3	0.3h
ARCHER2_CSE_Level2	55	68	32	12	0.2h
ARCHER2_CSE_Level3	2	0	3	0	0
ARCHER2_CSE_TA	8	7	1	8	0.3h
May 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	76	70	6	3	0.2h
ARCHER2_CSE_Level2	57	58	31	11	0.3h
ARCHER2_CSE_Level3	1	1	3	27	0.1h
ARCHER2_CSE_TA	3	3	1	9	0.2h
Jun 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	113	119	0	3	0.5h
ARCHER2_CSE_Level2	56	65	22	12	0.2h
ARCHER2_CSE_Level3	0	3	0	29	0.4h
ARCHER2_CSE_TA	3	4	0	9	0.3h
Q2 2024					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	341	347	0	3	0.3h
ARCHER2_CSE_Level2	168	191	22	12	0.2h
ARCHER2_CSE_Level3	3	4	0	29	0.3h
ARCHER2_CSE_TA	14	14	0	9	0.2h

CSE Query Categories

A total of 556 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	347	62.4%
ARCHER2_CSE_Level2	3rd party software	40	7.2%
	Batch system and queues	31	5.6%
	Compilers and system software	24	4.3%
	Software installation	23	4.1%
	eCSE applications/calls	14	2.5%
	Software errors	12	2.2%
	Login, passwords and ssh	10	1.8%
	Porting, performance and scaling	10	1.8%
	Courses	7	1.3%
	Storage and compute resources	7	1.3%
	Data transfer	6	1.1%
	Hardware issue	3	0.5%
	User behaviour: Queries relating to user behaviour	3	0.5%
	Website and documentation	1	0.2%
ARCHER2_CSE_Level3	3rd party software	2	0.4%
	Batch system and queues	1	0.2%
	Storage and compute resources	1	0.2%
ARCHER2_CSE_TA	Grant	12	2.2%
	Pump-priming	2	0.4%
Total		556	100.0%

ARCHER2 Training

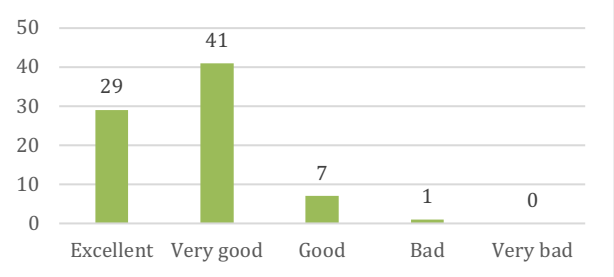
As part of ARCHER2, the service has been developing and delivering a training programme for the ARCHER2 community. During the second quarter of 2024, the CSE service has provided a total of 23 days of training, scheduled as follows:

Dates	Course	Location	Days	Attend
3-4 Apr	Introduction to Modern Fortran	Durham	2	5
3-4 Apr	MPI	Cambridge	2	15
8 Apr	Introduction to CP2K	Online	1	20
10-11 Apr	Modern C++	York	2	29
10-11 Apr	Intermediate Fortran	Edinburgh	2	13
15 Apr	Introduction to XCompact3D	London	1	14
16-17 Apr	Containers	Birmingham	2	18
18-19 Apr	GPU HIP	Online	2	25
29-30 Apr	Scalasca	Edinburgh	2	14
15 May	Developing in-situ analysis capabilities for pre-exascale simulations with Xcompact3D	Online	0.5	7
18-19 Jun	Introduction to Data Science and Machine Learning	Online	2	25
19-20 Jun	HPC Carpentry	Southampton	2	25
25 Jun	Introduction to Porting and Running Applications on AMD GPUs	Online	0.5	25
27-28 Jun	Advanced MPI	Online	2	17

We have initiated a collaboration with AMD and a series of training sessions will be delivered in order to upskill accelerator capabilities in the direction of Exascale computing. The first session was delivered as a webinar on the 25th of June.

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 4.3, i.e., better than "Very Good". Users provided 78 responses, a response rate of 35%.



ARCHER2 and GPU Embedded CSE Programme (eCSE)

ARCHER2 eCSE

The ARCHER2 eCSE programme awarded 806 PMs across 11 calls, exceeding the contractual requirement of 798 PMs. The table below shows the number of proposals received and the projects awarded across the programme.

ARCHER2 eCSE call	Call Dates	# Technical Evaluations Received	# Proposals Received (EPSRC,NERC)	# PM requested (EPSRC, NERC)	# Proposals accepted (EPSRC, NERC)	# PMs Awarded (EPSRC, NERC)
eCSE01	19/05/20 - 07/07/20	25	25 (25,0)	235 (235,0)	13 (13,0)	132 (132,0)
eCSE02	08/09/20 - 27/10/20	13	12 (9,3)	107 (87,20)	7 (4,3)	53 (33,20)
eCSE03	08/12/20 - 16/03/21	15	14 (10,4)	136 (105,31)	8 (6,2)	75 (56[1],19)
eCSE04	20/04/21 - 08/06/21	13	11 (7,4)	109 (83,26)	7 (4,3)	60 (37,23)
eCSE05	07/09/21 - 26/10/21	10	9 (9,0)	85 (85,0)	5 (5,0)	47 (47,0)
eCSE06	09/12/21 - 15/03/22	7	6 (6,0)	61 (61,0)	5 (5,0)	58 (58[2],0)
eCSE07	19/04/22 - 14/06/22	13	10 (10,0)	77 (77,0)	7 (7,0)	55 (55,0)
eCSE08	06/09/22- 25/10/22	17	12 (12,0)	144 (144,0)	7 (7,0)	82 (82[1],0)
eCSE09	06/12/22- 14/03/23	12	12 (12,0)	146 (146,0)	6 (6,0)	67 (67,0)
eCSE010	18/04/23 - 13/06/23	5	5 (5,0)	59 (59,0)	4 (4,0)	44 (44,0)
eCSE011	12/09/23 - 31/10/23	16	16 (16,0)	190 (190,0)	12 (12,0)	133 (133,0)
Total		**146**	**132 (121,11)**	**1349 (1272,77)**	**81 (73,8)**	**806 (744,62)**

[1] In both cases this includes 2 PMs extra being awarded within the original budget of a project. This was due to the staff member involved in each case incurring lower costs than expected as the individual had opted out of the University pension scheme.
[2] This includes 6 PMs extra awarded for a member of staff on maternity leave.

GPU eCSE

- The first of a new programme of GPU eCSE calls opened on 17/01/2024 and closed on 19/03/2024, receiving 51 proposals for the development of software within the remit of 5 different research councils (ESRC, EPSRC, STFC, NERC and MRC) requesting a total of 1182.8 person months.
- The panel meeting took place on 08/05/2024 and 8 projects were awarded funding awarding a total of 231.8 person months.
- The second GPU eCSE call opened on 02/07/24 and will close on 17/08/2024 for projects starting in the first half of 2025.

GPU Call	Number of proposals	Number of PMs requested	Number of proposals awarded	Number of PMs awarded
1st GPU eCSE call	51	1182.8	8	231.8

Early Career Observers call

An Early Career Observers call was opened alongside the 1st GPU software development call. The call gives early career researchers the opportunity to attend an eCSE panel meeting as observers. The most recent call received 11 applicants, all of whom were accepted to attend a panel meeting. These observers either attended the panel meeting for the first call or will be invited to attend the panel meeting for the second call.

ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Festivals and Workshops

The team delivered a workshop on the “Power of Programming” at the Edinburgh Science Festival (30 March–14 April). The children learnt how to program a micro:bit and simulate disease spread based on interactions with other micro:bits. They learnt a little about supercomputers and the sort of science done on them.

We attended the Big Bang Fair (19-21 June) at the NEC in Birmingham. Across the 3 days, over 20,000 secondary-aged children attended, and our booth was busy for the full event. The event ran smoothly with the children seemingly engaged and interested in the activities. Four activities were showcased:

- Wee Archie – running with a new framework, this allowed for a higher throughput and better graphics.
- Logic puzzles - Towers of Hanoi, Chicken, Grain and Fox, and Zombie escape. A "brute force" simulation, based on random numbers, was on display showing that a computer solves these puzzles in fractions of a second vs several minutes of thinking for a human.
- Hardware – Real examples of Supercomputing hardware including ARCHER and ARCHER2.
- Sock Sorting – an improved version of this hands-on sorting example, it replaced the solid colour beanbags with patterned socks to improve accessibility.

Work Experience

Across the summer we have a significant number of students visiting to carry out work experience. During this quarter we have had two groups of students.

James Richings supervised two, week-long, summer placement students (3-7 June and 24-28 June). The students completed the Python training from the software carpentries course before learning about Pytorch with simple, binary-classifier examples on ARCHER2 before moving on to their projects using Machine learning.

The Edinburg Science Festival team supervised three students (10-14 June) who looked to enhance the micro:bit workshop delivered at ESF. The students developed a new puzzle for the micro:bits and looked in more depth at communication.

Over the remainder of the summer, we have five students from the Nuffield Research Programme on 3 week placements and a further two students carrying out work experience for a week.

Diversity and Inclusivity

The CSE team has contributed to two significant Women in HPC activities during the period.

ISC’24 (Hamburg, 12th—16th May) is the first run of this international conference since Women in HPC became an official collaborative partner. Building on this relationship and chaired by Weronika Filinger, WHPC ran its most ambitious programme yet, including:

- A Solution Takeover Forum during the Exhibition Gala
- Diversity Day
- A poster and networking reception
- A Birds of a Feather on mentoring.

Participation in all of the events was very high: more details on the programme can be found in the WHPC's ISC Impact Report – 2024.

Outside of WHPC, Eleanor Broadway also organised and chaired an ISC BoF session on "HPC Outreach: Telling Our Stories of HPC in Science" and, along with Weronika Filinger, contributed presentations to a BoF on "Enhancing the Symbiosis Between HPC and RSE Communities."

Working with the N8 Women in HPC Chapter, Eleanor Broadway also helped organise a "WHPC: Community Building and Fostering Diversity" session at the Durham HPC/AI Days 2024. This session included four invited speakers and an interactive discussion with the audience to address lessons learned when building a community and how improving diversity improves the workplace. More details are available on the WHPC website.

Quality Management, Information Security and Business Continuity

EPCC recently passed our external audit for ISO 27001 (information security), ISO 9001 (quality service delivery) and ISO 22301 (business continuity).