ARCHER2 Quarterly Report

October – December 2022

EPCC

The University of Edinburgh

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ARCHER 2 Quarterly Report

This section of the report covers the period Oct 2022 – Dec 2022 for the ARCHER2 service.

ARCHER2 Executive Summary

- The CSE team has completed an evaluation of the Cray EX AMD GPU platform, in anticipation of the GPU component of ARCHER2 being delivered. This demonstrated that the environment could indeed be supported by the CSE team. The final report will be available early in the New Year, and further work will be carried out when clarity on delivery timescales is provided.
- Members of the CSE team have been looking at energy efficiency around the ARCHER2 service. The team successfully implemented a change to the default processor frequency, with early figures suggesting this has made a significant saving (600 MW/20%) to the power draw of ARCHER2.
- Progress has been made to understand the relatively poor performance of VASP on ARCHER2, one of the most heavily used codes on ARCHER2, and changes are expected in the next release of VASP to partially mitigate the issue.
- CSE contributed to EPCC securing ISO 22301 (Business Continuity) certification, which helps to ensure the service is ready to respond to significant incidents.
- The team had a booth at New Scientist Live in London in October, providing hands-on supercomputing-themed activities and educational content for the general public across 3 days.
- The CSE team made significant contributions to the Supercomputing 2023 programme, including helping to organise a full Women in HPC programme, the first full programme for three years (due to COVID difficulties).
- eCSE08 offered an increase from 12 person months to 18 person months per project with the intention of providing researchers with the opportunity to carry out more in-depth improvements to software and to allow for an increase in the scope of a project's objectives.
- Alongside the eCSE08 call, a call for early career researcher observers was launched (closing on 4/10/2022). The eCSE08 was attended by 3 such observers who gained a greater understanding of the selection process.
- A total of 15.5 days of online and face-to-face training have been delivered in this quarter. This included a face-to-face Software Carpentry workshop in Belfast, with an extended programme to meet the need for enhanced Python training.
- Women In HPC won the HPCwire Readers' Choice Award 2022 for Workforce Diversity, Inclusion and Leadership.

ARCHER2 Forward Look

- A significant focus for the team during the next quarter will be preparation for the software upgrade of ARCHER2. During this period the CSE team will have access to the upgraded TDS system and will utilise this to test and prepare applications for the full system upgrade.
- Members of the CSE team have been involved in a case study looking at ARCHER2's carbon footprint. This work is completing during this quarter however we plan to continue to investigate opportunities to reduce energy consumption going forward.
- Following the recent funding call for HEC Consortia, the CSE team will engage with the new consortium to ensure they are fully supported on the ARCHER2 system.
- EPCC has completed a recruitment round which will allow the CSE team to be expanded during January—June 2023.
- The eCSE09 call is open and we look forward to opening more calls beyond this given the recent extension to the CSE contract. The timetable is expected to follow a similar pattern as for previous calls.
- The CSE team are currently in the process of planning for the Edinburgh Science Festival, with a booth in the drop-in section of the National Museum of Scotland in April. This will allow members of the general public to enjoy hands-on activities showcasing Supercomputing.
- The ARCHER2 training programme for the fourth year of the ARCHER2 service will be designed in the upcoming quarter, considering the feedback from past delegates, the ARCHER2 Training Forum, and the ARCHER2 Training Panel, who will ultimately approve it.
- Planning for the International HPC Summer School 2023 is underway.

ARCHER2 Centralised CSE Team

This has been another productive period for the CSE Team, who have been able to take advantage of the further relaxation of Covid-19 restrictions to have more face-to-face interactions with the ARCHER2 (and wider HPC) community.

The team were represented at several HPC-relevant meetings and conferences during the period, as follows:

- Andy Turner, STFC in Conversation: Net Zero meeting, Hartree Centre, 24 Nov 2022
- Alan Simpson, Lorna Smith, Andy Turner, ARCHER2 User Advisory Group, Online, 28 Nov 2022
- Juan Rodriguez-Herrera, Andy Turner, CIUK, Manchester, 1–2 Dec 2022

and the following presentations:

- HPC-JEEP: job energy analysis, Andy Turner (EPCC) and Alastair Basden (Durham University), GoZero Workshop, Online, 5 Oct 2022
- HPC-JEEP: job energy analysis, Andy Turner (EPCC) and Alastair Basden (Durham University), CIUK, Manchester, 2 Dec 2022
- David Henty, "Parallel I/O performance on ARCHER2", EPCC - Tsukuba Collaboration Workshop, Edinburgh, 14—15 December 2022
- HPC-JEEP: job energy analysis, Andy Turner (EPCC) and Alastair Basden (Durham University), EPCC-Tsukuba Workshop, Edinburgh, 14 Dec 2022

The team was also well represented at the Supercomputing 2022 (SC) conference (Texas, 13—18 November). Two members of CSE (Eleanor Broadway and William Lucas) presented an invited talk on behalf of the team at the 'Research Software Engineers in HPC: Creating Community, Building Careers, Addressing Challenges' workshop on the Sunday of the conference. This talk discussed challenges addressed by the ARCHER2 CSE team including how to manage a mixed workload, how to share knowledge amongst a diverse team and how the team was impacted by remote/hybrid working. The talk was well-received and generated discussion in the room afterwards with members of teams at other sites in the US and elsewhere.

SC was also a good opportunity to meet members of the wider HPC community and catch up with latest developments and research in hardware and software. The CSE team also contributed to a full Women in HPC programme at SC, which is described later in this report.

Finally, the CSE team played an important role in the preparations for the external audit for our ISO22301 (Business Continuity) certification, including developing and operating key business-continuity processes.

EPCC has undertaken a major recruitment round during September—October and, as an output of this, we look forward to expanding the CSE team in 2023. Once on-boarded, the additional staff will provide greater capacity for progressing service improvement activities.

Continual Service Improvement (CSI) Projects

ARCHER2 GPU Evaluation

The CSE team (Michael Bareford, Larisa Stoltzfus, and Kevin Stratford) complete the evaluation of the Cray EX AMD GPU platform.

With the help of the HPE Centre of Excellence team, they were able to complete outstanding experiments, noted in the previous report, on a second internal HPE system called *Pinoak* (initially, the team were given access to an internal system called *Marvin 4*). Pinoak was not directly accessible to the team, but Douglas Shanks (CoE) built the remaining applications – NAMD and LAMMPS – and ran the benchmarks needed to complete the report.

Pinoak had a more complete development environment and some of the debugging/ profiling tests that had failed on Marvin 4, were more successful on Pinoak.

The final report from which will be available at the beginning of 2023.

VASP Performance Evaluation on ARCHER2

The CSE team have continued to work with the VASP development team at the University of Vienna to understand VASP performance on ARCHER2 and AMD EPYC CPUs more generally. This collaboration has led to an improvement in the benchmark cases used to investigate the problematic performance and some changes to the source code in the upcoming VASP 6.4 release to improve multi-threaded performance. The ongoing investigations indicate that the case where we saw poorer than expected performance may be memory-bound and that the reduced per-core memory bandwidth on ARCHER2 compared to ARCHER may explain some of the performance differences. Investigations are continuing and we hope to provide a technical report discussing the findings in the first half of 2023.

Evaluation of the Cray Containerised Programming Environment

The HPE-led evaluation of a containerised version of the Cray Programming Environment has also wrapped up. HPE has confirmed that, from 2023, they will release the necessary artefacts for building the CPE containers, as opposed to releasing a complete (Docker) container image.

The CSE team (primarily, Michael Bareford and Andy Turner) engaged with the evaluation throughout, and are well placed to formalise a strategy for providing access to CPE containers for ARCHER2 users during 2023.

Package Management with Spack

Due to other team commitments, progress to develop the processes and policies for using Spack to manage software packages on ARCHER2 has been limited. With the addition of new staff, in 2023Q1, we expect to be able to invest the time needed to complete this work then.

ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from October 2022 – December 2022. The metrics were specified by UKRI in the ARCHER2 CSE 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 OY3: Service Threshold: >4.2 WD; Operating Service Level: >1.2 WD, ≤2.2 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 OY3: Service Threshold: >26 Working Days (WD); Operating Service Level: >11 WD, ≤16 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 OY3: Service Threshold: >57 Working Days (WD); Operating Service Level: >27 WD, ≤37 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 OY3: 7 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 2022		Nov 2022		Dec 2022		Q4 2022	
	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)	1.2WD	-2	0.3WD	-2	0.7WD	-2	0.8WD	-6
ARCHER2_CSE_Level3 (MTR)	1.4WD	-2	-		10WD	-2	6WD	-4
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	96.2%	-2	95%	-2	97.3%	-6
Training Satisfaction (%)			100%	-1	100%	-1		-2
Total		-10		-9		-11		-30

380 query feedback responses were received on query resolution in the Reporting Period. 97.3% 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 2022 – December 2022.

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 2022					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	28	28	0	3	0.4h
ARCHER2_CSE_Level2	47	56	14	12	0.3h
ARCHER2_CSE_Level3	1	1	3	35	0.2h
ARCHER2_CSE_TA	5	8	0	8	0.2h
Nov 2022					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	158	152	6	4	0.4h
ARCHER2_CSE_Level2	54	42	26	12	0.2h
ARCHER2_CSE_Level3	2	0	5	0	0
ARCHER2_CSE_TA	6	3	3	10	0.4h
Dec 2022					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	33	39	0	4	0.5h
ARCHER2_CSE_Level2	38	46	18	13	0.2h
ARCHER2_CSE_Level3	1	1	5	23	0.2h
ARCHER2_CSE_TA	1	4	0	11	0.8h
Q4 2022					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1	219	219	0	4	0.4h
ARCHER2_CSE_Level2	139	144	18	12	0.2h
ARCHER2_CSE_Level3	4	2	5	29	0.2h
ARCHER2_CSE_TA	12	15	0	9	0.4h

CSE Query Categories

A total of 380 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	219	57.6%
ARCHER2_CSE_Level2	3rd party software	52	13.7%
	eCSE applications/calls	28	7.4%
	Batch system and queues	20	5.3%
	Courses	11	2.9%
	Access to services	7	1.8%
	Data transfer	5	1.3%
	Compilers and system software	4	1.1%
	Login, passwords and ssh	4	1.1%
	Porting, performance and scaling	4	1.1%
	Software errors	4	1.1%
	Software installation	2	0.5%
	Storage and compute resources	2	0.5%
	Hardware issue	1	0.3%
ARCHER2_CSE_Level3	3rd party software	2	0.5%
ARCHER2_CSE_TA	Pump-priming	7	1.8%
	UKRI Grant	5	1.3%
	Fellowship	2	0.5%
	Access to HPC	1	0.3%
Total		380	100%

ARCHER2 Training

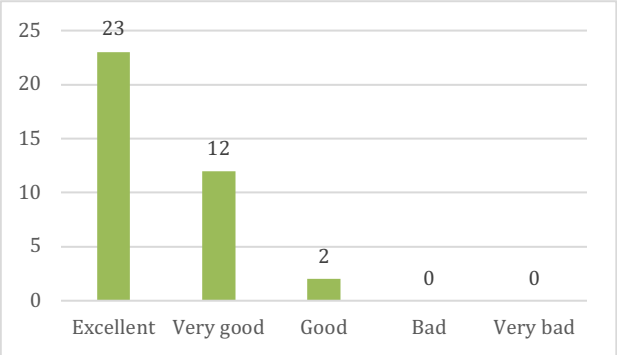
As part of ARCHER2, the service has been developing and delivering a training programme for the ARCHER2 community. During the last quarter of 2022, the CSE service provided a total of 15.5 days of training, scheduled as follows:

Dates	Course	Days	Attend
2 Nov 2022	Debugging on ARCHER2: Introduction to the gdb4hpc and ccdb debugging tools on ARCHER2	0.5	40
24 Nov 2022	ARCHER2 for Package Users	1	10
29-30 Nov 2022	Advanced OpenMP	2	17
2, 5 Dec 2022	ARCHER2 for Software Developers	2	7
5-8 Dec 2022	Software Carpentry	3.5	27
7-8 Dec 2022	Reproducible computational environments using containers	2	20
7 Dec 2022	Application programming interface for density functional theory software	0.5	18
13-14 Dec 2022	Introduction to Modern Fortran	2	19
13-14 Dec 2022	Performance Optimisation on AMD EPYC	2	12

The Software Carpentry workshop took place in Belfast. The format was longer than the standard two-day duration in order to include more lessons and spend more time on the Python lesson.

Due to a train strike, the "Introduction to Modern Fortran" course was switched to an online format after a poll was run among the registered people. The online format was more popular, and the number of registrations notably increased.

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 37 responses, a response rate of 35%.



ARCHER2 Embedded CSE Programme (eCSE)

eCSE calls 1-9

- Call 8 (eCSE08) opened on 6/09/2022 and closed for technical evaluations on 4/10/2022 receiving 17 documents for technical evaluation. The call finally closed on 25/10/2022 receiving 12 submissions. The panel meeting for the eCSE08 call took place on 14/12/2022. 7 of the 12 proposals were accepted to become projects with 80 person-months awarded overall.
- For eCSE08, proposals were invited for up to 18 person months per project (an increase from 12). This increase in effort was intended to provide researchers with the opportunity to carry out more in-depth improvements to software and to allow for an increase in the scope of a project's objectives.
    - Of the 12 proposals received, 3 proposals did request more than 12 PMs (1 project requested 15 PMs and 2 requested 18 PMs). Of these, one project (with 18 PMs) was awarded funding. We will monitor the progress of the project to determine if any issues arise due to the longer length.
- For call 1 and from call 5 onwards, only proposals with software within the EPSRC remit have been eligible.
- Call 9 (eCSE09) opened on 6/12/2022 and closes for technical evaluations on 21/02/2023 with a final deadline for the call of 14/03/2023.
    - As for eCSE08, the call is open for projects of up to 18 PMs.

eCSE call	Call Dates	# Technical Evaluations Received	# Proposals Received (EPSRC,NERC)	# PM required (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)	73 (54,19)
eCSE04	20/04/21 - 08/06/21	13	12 (9,3)	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)	49 (49,0)
eCSE07	19/04/21 - 14/05/22	13	10 (10,0)	77 (77,0)	7(7,0)	55(55,0)
eCSE08	6/09/22- 25/10/22	17	12(12,0)	144(144,0)	7(7,0)	80(80,0)
Total		**113**	**100 (90,10)**	**954 (877,77)**	**59 (51,8)**	**549(487,62)**

ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Blogs

The service continues to publish regular blog articles, highlighting different aspects of the work carried out by the CSE service. These include a blog around the software power draw on ARCHER2 and the Impact of CPU frequency on application performance on ARCHER2.

Community and Outreach Activities

The CSE team had a booth at the New Scientist Live 2022 event (London, 7—9 October). The team presented interactive activities to showcase the importance of supercomputing including real hardware from ARCHER2, logic puzzles, a ball-sorting activity, and Wee Archie, the "suitcase-sized" supercomputer.

EPCC were involved in an outreach Birds of a Feather session at SC22, titled Another step toward a Sustainable HPC Outreach Ecosystem. The BoF committee members expressed an interest to run a similar session at ISC23.

Diversity and Inclusivity

Women in HPC ran a full programme of activities at Supercomputing 2022 (for the first time in three years), including a workshop on diversifying the HPC community and engaging allies (co-organised by Weronika Fillinger), and a networking reception. WHPC also organised a Diversity Day campaign for Tuesday 15th November. George Beckett helped organise fund-raising and financing for the programme.

Figure 1: SC22 WHPC Workshop Contributors and Participants

The programme culminated in Women in HPC being awarded the HPCwire 2022 Readers' Choice award in the Workforce Diversity, Inclusion and Leadership category.

Planning for WHPC workshops at ISC23 and SC23 has started (submissions are due on 19 January and 24 February, respectively). Weronika Filinger and the new EPCC Chapter co-chair (Eleanor Broadway) are members of the relevant organising committees.

Planning for the International HPC Summer School 2023 (https://ss23.ihpcss.org/) stated in late September. The event will take place in Atlanta, during 9th—14th July. The call for participation has been

opened on December 12th and will close on January 31st. For the first time the school will also include participants from Australia and South Africa. Work on the new agenda (reflecting the feedback from the previous event) has started as well. Ludovic Capelli will teach the GPU programming track, David Henty will cover the MPI track, and Weronika Filinger will run the mentoring programme.

Work continues for the ACM SIGHPC Education Chapter. The chapter officers and committee chairs met at SC22 to plan activities for 2023. The first ACM SIGHPC Education Award for Outstanding Contribution to Computation Science Education was presented at SC22 during the Thursday Award Ceremony. Looking forward, planning for the ISC23 and SC23 workshops (HPC Education and Training for Emerging Technologies) are ongoing.