ARCHER2 Quarterly Report

January—March 2024

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0.2	2024-03-29	ARCHER2 CSE queries performance report, statistics and analysis added.	Xu Guo
0.3	2024-04-05	Added info on audits, blogs and benefits realisation	Anne Whiting
0.4	2024-04-08	eCSE updates	Chris Johnson
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ARCHER 2 Quarterly Report

This report covers the period January–March 2024 for the ARCHER2 service.

ARCHER2 Executive Summary

- The ARCHER2 team ran a well-received and positive Celebration of Science event on 7⁻8 March in Edinburgh. The event had around 90 attendees and showcased the diverse range of science being delivered by the service.
- Women in HPC held a successful and interactive workshop, co-located with the ARCHER2 Celebration of Science, which highlighted the benefits of diversity to research on 8 March.
- The first eCSE fund, which funded software targeted at ARCHER2, has been allocated and the required PM count exceeded. In total 81 separate projects have been funded with this money, delivering improvements to the software base across a range of science areas.
- The second set of eCSE funding targets GPU development and has been expanded to all UKRI research councils. This provides opportunities for RSEs to develop skills and for the community to prepare for future platforms. The first call has recently closed and is currently in the review stage.
- The ARCHER2 GPU development system was launched in early February and the CSE team has spent significant time this quarter setting up and testing the system for user service. This included running a webinar, providing an initial suite of software and developing documentation to promote uptake.
- The CSE team also lead the development of the Capability Days programme, which ran for the first time in March, incentivising users to experiment with capability-scale workloads. Interest was high and plans are being put in place to run further Capability Days.
- The CSE service has provided a total of 23.5 days of training this quarter. The training team has also been developing the training plan for the coming year, gaining input from the community at the User Forum and at the training Forum.
- Women in HPC has relaunched its mentorship programme. This has been very well received with more than 30 applications. Successful applicants will work on a programme of activities culminating in ISC'24.
- The outreach team have been developing new materials for a workshop at the Edinburgh Science Festival, which introduces programming to children and highlights the importance of computer simulation in a fun and interactive way using micro:bits.

ARCHER2 Forward Look

- Final preparations are being made for our annual ISO external audit in June. This will cover all 3 standards, ISO 9001 for quality service delivery, ISO 27001 for information security and ISO 22301 for business continuity and disaster recovery. Our external audit reviews our work against the standards to ensure that we are complying with what is required and continue to apply best practice.
- The panel meeting for the first call of the new GPU eCSE programme is expected to take place in early May to decide on the first group of proposals to fund. Most projects are then expected to start between May and September. We expect to open a further call in June.
- The training program will continue with new courses covering the ARCHER2 AMD GPU development platform due to be delivered.
- Members of the CSE team will be at CUG'24, presenting work from the ARCHER2 service and sharing best practice with other large-scale HPE sites. CSE staff will also be present at ISC'24, again sharing best practices. Both Wee Archie and the VR tour of ARCHER2 will be on display on the EPCC booth in the ISC'24 exhibit hall, showcasing the service to the wider community.
- The ARCHER2 team will present a workshop at the Edinburgh Science Festival, providing a fun and hands-on experience of programming. During this quarter the team will also be preparing for the Big Bang Fair in June in Birmingham.
- The plan is to run another Capability Day during this quarter and preparations are underway to provide the best possible experience for users.
- WHPC has a full programme of EDI activities planned for ISC'24.

ARCHER2 Centralised CSE Team

It has been a busy and productive quarter for the CSE team, which began with the setup and testing of the ARCHER2 GPU Development Service in preparation for a launch at the beginning of February. The CSE team ran a webinar to support the introduction, plus provided both introductory training and an initial suite of software and documentation to promote uptake. Further, from April, the licence for the Linaro Forge development tools has been extended to cover the GPU system too.

The introduction of the GPU Development service was timely, coinciding with the launch of the new eCSE GPU programme, discussed later in this report.

The CSE team also lead the development of the Capability Days programme, which ran for the first time in March, incentivising users to experiment with capability-scale workloads both to exploit the unique potential of ARCHER2 as a Tier 1 service and to grow community experience with larger-scale research computing in preparation for the Exascale Pathway system. A report on the initial run of the Capability Days scheme has been produced and shared with the ARCHER2 stakeholders.

The CSE team (as well as the SP team) were well-represented at the STFC Exascale Requirements workshop on 14th March, with George Beckett, James Richings, and Jo Beech-Brandt contributing to the event.

The CSE team ran several webinars during the period:
- Introducing the ARCHER2 GPU service (Turner)
- ARCHER2 GPU eCSE software development call webinar (Johnson and Smith)
- Visualisation: Paraview and Blender (Lemaire)
- Parallel IO profiling (Parisi)
- Introduction to capability days (Turner and Stratford)

Several high-profile conferences will be held in the coming months and the CSE team has begun preparations for contributing to these. First, the CUG'24 conference is being hosted by the Pawsey Centre, in Perth, Australia, in May. ARCHER2 will be represented by Juan Rodriguez-Herrera (who is also an elected member of the CUG Board) and Adrian Jackson. Juan will present a paper on "Scalability and Performance of OFI and UCX on ARCHER2", coauthored with Michael Bareford, Evgenij Belikov and Jaffery Irudayasamy.

Soon after CUG is the International Supercomputing Conference (ISC) which, this year, is a little earlier than usual being held in Hamburg, Germany, during 12th—16th May. The CSE team has a number of contributions:
- Andy Turner and Eleanor Broadway are contributing to an RSEHPC Workshop (https://www.rse-hpc.org/).
- Eleanor Broadway has an accepted Birds of a Feather session on Telling the Story of HPC in Science.
- Weronika Filinger also has a Birds of a Feather session on Developing a Sustainable Future for HPC and RSE Skills: Training Pathways and Structures and she is giving a workshop talk on "UNIVERSE-HPC - Defining MSc programme for RSEs in HPC"
- Further, in the run-up to the conference, George Beckett was part of the selection panel for the ISC poster competition, which received a record number (eighty-five) submissions for judging.

Women In HPC – now an official ISC collaborator – has a full programme of activities and engagement opportunities at ISC, which are described in more detail later in the report.

Closer to home, Andy Turner participated in the CP9 Conference (Chester, 19-22 Mar 2024), presenting on ARCHER2 and national HPC.

Looking further forward, Eleanor Broadway is part of the committee for the SC24 Reproducibility Challenge, reviewing papers from SC23 to identify a candidate to reproduce during the Student Cluster Competition. Eleanor is also part of the programme committee for the PERMAVOST workshop (4th Workshop on Performance EngineeRing, Modelling, Analysis, and VisualizatiOn STrategy), being held in Italy during 3rd—4th June 2024.

Continual Service Improvement (CSI) Projects

Supported Software on the ARCHER2 GPU Development System

To widen the scope of potential user experimentation with the ARCHER2 GPU Development System, the CSE team is configuring GPU versions of a subset of the supported software, based on anticipated interest and software readiness.

The PyTorch machine-learning framework has been extended to work on the GPU nodes (in addition to CPU nodes, already available). Initial benchmarking has been successfully completed and, once CSE testing is complete, it will be made available to users.

Work is also on-going to port Tensorflow, which is a peer of PyTorch, though there are some challenges still to be resolved.

Moving forward, LAMMPS, VASP, NEMO, CASTEP, OpenSBLI and GROMACS will also be extended and benchmarked on the GPU nodes.

Spack Package Management on ARCHER2

The CSE team has continued to develop a strategy for using the Spack Package Management system to simplify and streamline scientific software deployments on ARCHER2. At the time of writing, a candidate configuration of Spack has been successfully tested with several of the CSE supported software packages on ARCHER2 and has been made available to the wider CSE team for further testing. All going well, the use of Spack for a significant portion of the CSE supported software should be in place by the Summer.

Scalability and Performance of OFI and UCX on ARCHER2

The choice of OFI versus UCX as the communication framework on which to run user jobs is a challenging one for users with mixed evidence as to which is more reliable or performant for different simulation types and sizes. Aiming to grow the understanding of this choice, the CSE team (led by Evgenij Belikov) is refreshing and extending a study of OFI and UCX undertaken at the beginning of the (four-cabinet) ARCHER2 service (M. Bareford, D. Henty, W. Lucas, and A. Turner, "OpenFabrics and UCX: Performance on the ARCHER2 HPE Cray EX system," CUG 2022) and taking into account performance on the full ARCHER2 system and improvements in the HPE-provided software stack (particularly, the Slingshot software).

The work has been accepted as a paper for CUG 2024 and the results will be useful to formulate better guidance for users, as part of the ARCHER2 documentation.

Quantum Simulations

The ARCHER2 team provided a tour of the ACF to the head of the National Quantum Computing Centre; and outlined recent use of ARCHER2 for large-scale quantum simulation workloads as well as options for future collaboration.

The CSE team (specifically, James Richings and Oliver Brown) continues to grow the collaboration with the Quantum Software laboratory in University of Edinburgh School of informatics, which is likely to lead to further opportunities in the field of quantum computing.

Expansion of Reframe Test Coverage

EPCC intern, Chris Rae, has been extending the ARCHER2 (and Cirrus) Reframe suite to include the "mlperf" and "mlperfhpc" benchmarks, covering both the ARCHER2 CPU and GPU nodes. Chris will present the work at the Durham HPC days event in May (as part of the Talent Pipeline for HPC track) and has also submitted a paper on the project to the PERMAVOST workshop (noted above).

Chris is planning to look at options to optimise ML frameworks, based on the work to date, and to use the outputs to help train others on ML framework implementations and performance.

ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from January 2024 – March 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 OY4: Service Threshold: >4.1 WD; Operating Service Level: >1.1 WD, ≤2.1 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 OY4: Service Threshold: >25.5 Working Days (WD); Operating Service Level: >10.5 WD, ≤15.5 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 OY4: Service Threshold: >56 Working Days (WD); Operating Service Level: >26 WD, ≤36 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 OY4: 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	Jan 2024		Feb 2024		Mar 2024		Q1 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)	0.4WD	-2	0.6WD	-2	0.9WD	-2	0.6WD	-6
ARCHER2_CSE_Level3 (MTR)	-		20WD	-0.5	28WD	0	23WD	-0.5
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	97.6%	-2	99.1%	-6
Training Satisfaction (%)	96.77%	-0.25	100%	-1	100%	-1	97.96%	-2.25
Total		-8.25		-9.5		-9		-26.75

111 query feedback responses were received on query resolution in the Reporting Period. 99.1% of responses had a score of "Good", "Very Good" or "Excellent". All feedback rated less than good is reviewed by management and improvement actions taken as appropriate.

ARCHER2 CSE Queries

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

Jan 2024					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	236	235	1	3	0.4h
ARCHER2_CSE_Level2	69	61	32	11	0.4h
ARCHER2_CSE_Level3	4	0	4	0	-
ARCHER2_CSE_TA	4	2	2	7	0.2h
Feb 2024					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	136	137	0	3	0.3h
ARCHER2_CSE_Level2	106	81	57	11	0.4h
ARCHER2_CSE_Level3	0	3	1	20	0.2h
ARCHER2_CSE_TA	5	6	1	9	0.2h
Mar 2024					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	168	168	0	3	0.4h
ARCHER2_CSE_Level2	101	114	44	11	0.2h
ARCHER2_CSE_Level3	0	1	0	24	0.2h
ARCHER2_CSE_TA	4	4	1	8	0.6h
Q1 2024					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	540	540	0	3.178	0.4h
ARCHER2_CSE_Level2	276	256	44	11.16	0.3h
ARCHER2_CSE_Level3	4	4	0	21.25	0.2h
ARCHER2_CSE_TA	13	12	1	8	0.3h

CSE Query Categories

A total of 812 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	540	66.5%
ARCHER2_CSE_Level2	eCSE applications/calls	53	6.5%
	3rd party software	47	5.8%
	Batch system and queues	34	4.2%
	Software installation	23	2.8%
	Courses	18	2.2%
	Login, passwords and ssh	18	2.2%
	Compilers and system software	17	2.1%
	Software errors	17	2.1%
	Porting, performance and scaling	10	1.2%
	Data transfer	6	0.7%
	Storage and compute resources	5	0.6%
	Access to services	3	0.4%
	Hardware issue	2	0.2%
	Website and documentation	2	0.2%
	Other: Queries which do not fit within other categories	1	0.1%
ARCHER2_CSE_Level3	Software errors	2	0.2%
	3rd party software	1	0.1%
	Login, passwords and ssh	1	0.1%
ARCHER2_CSE_TA	Grant	8	1.0%
	Pump-priming	4	0.5%
Total		812	100.0%

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ARCHER2 Training

As part of ARCHER2, the service has been developing and delivering a training programme for the ARCHER2 community. During the first quarter of 2024, the CSE service has provided a total of 23.5 days of training, scheduled as follows:

Dates	Course	Location	Days	Attend
17 Jan	Advanced LAMMPS	Online	1	23
18-19 Jan	HPC Carpentry	Liverpool	2	27
23-24 Jan	Advanced OpenMP	Online	2	10
23-25 Jan	Software Carpentry	Newcastle	3	20
30-31 Jan	Introduction to Data Science and Machine Learning	Online	2	29
31 Jan	ARCHER2 GPUs	Online	0.5	68
7-8 Feb	Data Analysis and Visualisation in Python	Online	2	23
8 Feb	ARCHER2 GPU eCSE software development call	Online	0.5	38
12-15 Feb	Data Carpentry	Online	2	8
14 Feb	Using Blender for Scientific Visualisation	Online	0.5	66
21 Feb	Understanding parallel I/O perf. through profiling	Online	0.5	28
22-23 Feb	HPC Carpentry	Brunel	2	15
26-27 Feb	Modern C++ for Computational Scientists	Online	2	29
28 Feb	ARCHER2 Capability Days	Online	0.5	11
4 Mar	ARCHER2 for Data Scientists	Online	1	14
12-13 Mar	Overview of the ARCHER2 GPU Dev. Platform	Online	2	15

In collaboration with HPE Cray Centre of Excellence, we delivered the first course on the ARCHER2 AMD GPU development platform. The course was attended by some members of the CSE team as well as members of the ARCHER2 community. This course is the first of a series of courses covering the aspects needed to use a GPU as a developer or research package user.

On the feedback for 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 4.2, i.e., better than "Very Good". Users provided 98 responses, a response rate of 46%.
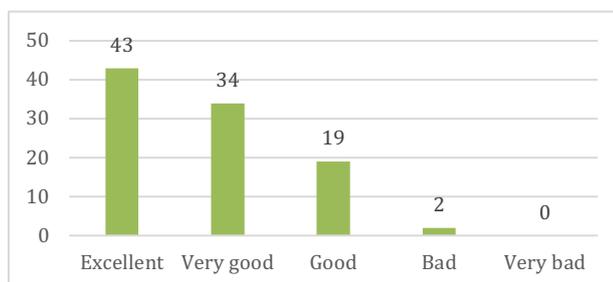
ARCHER2 Embedded CSE Programme (eCSE)

- eCSE calls 1-11
  - The eCSE programme has awarded 806 PMs across 11 calls. The contractual requirement was the award of 798 PMs meaning that the programme has now exceeded the required number of PMs and no further ARCHER2 eCSE calls are expected to be opened in the near future.
- eCSE 1st GPU call
  - 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 4 different research councils (ESRC, EPSRC, STFC, NERC and MRC). A panel meeting is expected to take place in early May to determine which proposals to fund.
- 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 the eCSE panel meeting as observers. This call received 11 applicants, all of whom will be invited to an upcoming panel meeting alongside any successful applicants from previous calls.

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)	59 (59,0)	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.

The graph below shows the current person months awarded to eCSE projects to date (blue line) along with the number to be awarded for the first 4 years of ARCHER2 (orange line).

eCSE person month spend against time
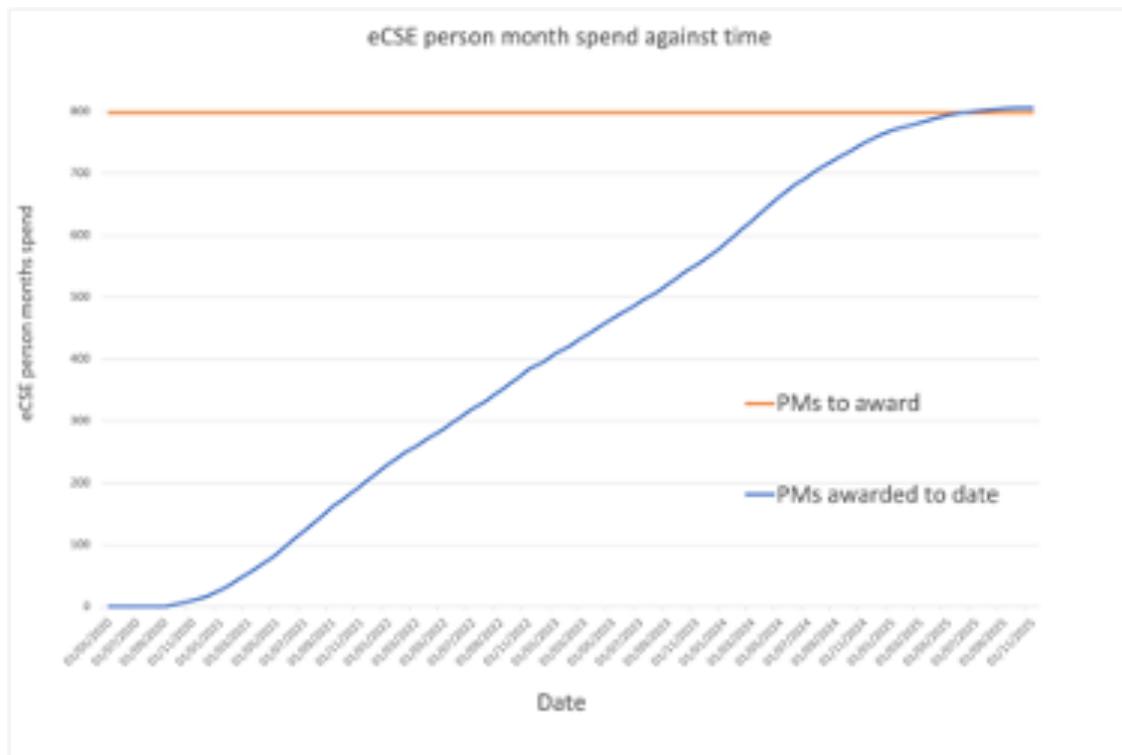
ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Benefits Realisation

Benefits realisation data continues to be collected using the data supplied by our users in the SAFE and other service data such as jobs run. The aim of the collected and analysed data is to contribute to the business case for future investment in HPC for scientific research. All data is provided as summary statistics without any identifiable personal data and complies with the privacy statements shown at https://www.archer2.ac.uk/about/policies/.

Blogs

Seven blogs have been published this quarter and can be seen at https://www.archer2.ac.uk/about/news/blog. Highlights included a virtual tour of ARCHER2, further details from our Image Competition calendar entries, and reviews of the RSE Meetup and the ARCHER2 Celebration of Science.

Celebration of Science

The Celebration of Science took place on the 7th and 8th March in Edinburgh. The meeting was well received and had over 90 registrations. The event was an opportunity to meet up with a wide range of people involved in the ARCHER2 community, and to hear a range of presentations by some of the Consortia Leaders, PIs and other researchers benefitting from access to ARCHER2, and also from some of those involved in providing the ARCHER2 service. The event showcased the best of the Science being delivered on ARCHER2 with the poster session proving a highlight of the event, with 25 posters demonstrating their work on ARCHER2. Women in HPC held a successful and interactive workshop, co-located with the ARCHER2 Celebration of Science (see below for more details).

Diversity and Inclusivity

Women In HPC has resumed running the WHPC Mentoring Programme, with significant support from Jay Lofstead (Sandia National Labs, USA). The programme received more than 30 applications and successful applicants will work on a programme of activities culminating in ISC'24.

On International Women's Day (8th March), Eleanor Broadway and Weronika Filinger (from CSE) working with Jenny Wong (from 2i2C) organised a WHPC co-located event at the ARCHER2 Celebration of Science, titled "Diversity in Science". This event opened the floor to the audience to develop ideas for small but meaningful changes to benefit their local communities. The event was wrapped up with an informal networking session to continue the conversations and encourage further connections. The event was very well received with a summary of findings to be published on the WHPC website (www.womeninhpc.org).

Looking forward, the Women in HPC team is focused on preparations for an ambitious programme at ISC'24 (https://womeninhpc.org/events/isc-2024), including a Solution Forum Takeover at the Exhibitor Gala, an early-career poster session, and a Birds of a Feather session on Engaging in Mentorship, along with a publicity push for the celebration of diversity day on the first full day of the conference (14th May).

Further forward, CSE team member, Weronika Filinger, has been invited to talk at a mini-symposium session at the PASC'24 conference in Zurich at the beginning of June, on the topic of "Ethical and Societal Considerations in HPC Education and Training".

Quality Management, Information Security and Business Continuity

Preparation continues for our annual ISO external audit, which this year takes place in June, 3 months earlier than usual. We are updating the Information Security Management System to the latest version of ISO 27001. This not surprisingly has a much greater emphasis on cybersecurity and reflects the changes in the information security landscape since the standard was last updated 10 years ago. The audit covers three ISO standards, ISO9001 for quality service delivery, ISO 27001 for information security and ISO 22301 for business continuity and disaster recovery. Our continuing work on standards and certifications reflects the importance we put on keeping our users' data safe and delivering the highest level of service.