



# ARCHER2 CSE Quarterly Report

January - March 2023

EPCC

The University of Edinburgh



## Document Information and Version History

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## ARCHER 2 CSE Quarterly Report

This section of the report covers the period January 2023 – March 2023 for the ARCHER2 service.

### ARCHER2 Executive Summary

- A considerable focus for this quarter has been on completing an evaluation of the proposed new system software stack from HPE, using the TDS. Representatives from the EPSRC HEC and NERC Consortia have also had access to test the software stack.
- A technical report has been published detailing the CSE team's evaluation of the AMD GPU technology that is expected to be added to ARCHER2 service in due course.
- A further technical report has been published, looking at automated service monitoring for ARCHER2.
- A total of 12.5 days of online and face-to-face training have been delivered during the first quarter of the year. This included a face-to-face Software Carpentry workshop in Cardiff and a three-day MPI course at Imperial College, London.
- The ARCHER2 training forum meeting was held online at the beginning of March and was open to all users. The draft training programme was presented to the audience and future topics were discussed. Attendees were keen to see several courses on programming languages such as C++ and Fortran.
- This quarter has been a busy one for blogs with eight published, ranging from the very technical, examining the use of the Rust programming language and the science of the ARCHER2 Image Competition winners, to the experience of being an eCSE Early Career Observer.
- Three new case studies have been published, ranging from airborne pathogen spread, to coral reef transportation by ocean currents to flow within and around a windfarm.
- The team has a booth at the Edinburgh Science Festival and will host drop-in sessions at the National Museum of Scotland from 10-13 April. During this quarter the team have been preparing hands-on activities with new activities related to switches, circuits and binary numbers.
- From the eCSE08 call onwards we have offered an increase in the maximum size from 12 person months to 18 person months per project. The intentions of this are 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. This has proved valuable with the eCSE08 and eCSE09 calls each received 3 proposals requesting greater than 12 months.
- A pilot of a restructuring of the CSE team, aimed to disseminate more responsibilities to staff and to avoid individuals working on activities in isolation, is going well.

## ARCHER2 Forward Look

- The anticipated software upgrade is due in the next quarter and the team will continue to prepare for this upgrade. In particular the team will focus on providing the best support for users when accessing the upgraded system, to ensure we are able to return to a full service as quickly as possible.
- We are now in the early stages of the fourth year of the ARCHER2 training programme, and are planning a greater number of face-to-face courses to provide users with the greatest flexibility and opportunity to access courses in the format they prefer.
- We will continue to develop and release new case studies based on the high quality science being carried out on the ARCHER2 system.
- This quarter sees the team at the Edinburgh Science Festival, where we aim to engage families in computational science and showcase the value of Supercomputing to society.
- Nearly all the early career observers accepted at recent calls have now attended an eCSE panel meeting and feedback has been very positive. A further call will be opened alongside the next eCSE call to give even more early career researchers this opportunity.
- The CSE team expects to be able to share an analysis of the impact of the default clock-frequency change on ARCHER2 in the next reporting period.
- The CSE team will have a strong representation at the upcoming Cray User Group meeting (Helsinki, May '23), presenting work around energy efficiency and Slurm innovations.
- The CSE team is contributing to a full programme of activities by Women in HPC at the ISC'23 conference, looking to highlight and showcase diversity within HPC.
- The team has been working to offer tours of the ACF to members of the HPC community and beyond. To date a series of tours have taken place, with the focus for this quarter on developing a tour appropriate for upper secondary school children.
- We are preparing for a group of work experience students to join us for 2-3 weeks during the summer break, as part of the Nuffield Research Placement scheme from the Nuffield Foundation.

## ARCHER2 Centralised CSE Team

During this period, we have welcomed three new team members (from a recruitment round in late 2022): Rui Apostolo, Sebastien Lemaire, and Luca Parisi. After a short induction period, they are now fully participating in CSE activities.

We also piloted a restructuring of the team, during the period, prompted by feedback received from staff during a service review late last year. From 1<sup>st</sup> February, we set up three subteams within the CSE to deal with: CSE in-depth queries, training, and service improvements. Each team has four or five members who work together on topical requirements for their respective area. Teams rotate every three months, so each CSE member gets an opportunity to work on each service area. The motivation for this restructuring was three-fold: provide staff with more autonomy and responsibility for specific elements of CSE service delivery; to allow staff to work together on tasks; and, to give staff more time to focus on individual tasks. Early feedback suggests the restructuring has gone well. More formal feedback will be collected during April, based on which a decision on whether to continue with the new team structure will be made.

A focus for the CSE team, during the period, has been the evaluation of a prospective new ARCHER2 software stack on the TDS. The team has been checking functionality, robustness, and performance of the new staff, with feedback being incorporated into the recommendation on how to proceed with the update. The team has also welcomed key contacts from the HEC and NERC collaborations onto the TDS, to validate critical workflows and to prepare for the upgrade.

CSE staff were well represented at community events during the period. Of particular note:

- Michael Bareford presented at the [SIAM CSE Conference](#) (Amsterdam, 23rd February - 3rd March 2023) on *Community Software Usage on ARCHER2*
- James Richings represented ARCHER2 at the HPC-SIG meeting (Southampton, 6<sup>th</sup>—7<sup>th</sup> March 2023) including contributing to a lightning-talk session.

The CSE has made another successful round of submissions to the Cray User Group meeting, which is being held in Helsinki during 7<sup>th</sup>—11<sup>th</sup> May. The CSE team has three accepted contributions:

- A presentation on ARCHER2 energy efficiency (A. Jackson, A. Turner, and A. Simpson)
- A birds-of-a-feather session on energy-based charging – led by Andrew Turner, and including contributions from NERSC, HLRS, Pawsey, HPE.
- A presentation on the ReFrame testing framework, jointly developed by Juan Rodriguez-Herrera in collaboration with peers from CSCS.

During the period, one of the CSE team (James Richings) collaborated with a University of Edinburgh Chancellor's Fellow (Oliver Brown) to investigate the interaction of HPC and quantum computing. With guidance from Oliver, James was able to successfully simulate a 43-Qubit quantum computer, running on 2,048 ARCHER2 nodes using QuEST. This is believed to be one of the largest quantum-computer simulations achieved to date anywhere. The pair hope to soon run a 44-qubit simulation on 4,096 nodes, matching the achievement of the QuEST developers themselves. The size of these simulations scales exponentially in the problem size, so ARCHER2's demonstrated capability is highly valuable to quantum algorithm developers.

## Continual Service Improvement (CSI) Projects

### ARCHER2 GPU Evaluation

The CSE team (Michael Bareford, Larisa Stoltzfus, and Kevin Stratford) published a technical report based on the evaluation of the Cray EX AMD GPU platform undertaken in 2022 (<https://zenodo.org/record/7752810>). A copy of the report has been uploaded to the ARCHER2 website. This concluded the evaluation of the AMD GPU platform for now, though further work may be warranted once the position on the ARCHER2 GPU provision is clarified.

### **ARCHER2 Reframe Enhancements**

The Service Improvement Team has refreshed and extended the Reframe test suite, used to validate the user configuration of ARCHER2, in support of the evaluation of the new HPE system software stack, labelled Papaya+. This included upgrading to a major new version (Reframe Version 4.0), adding further application benchmarks, and introducing tests related to energy use of jobs. The work was the basis of a lightning presentation, given by James Richings, at the HPC-SIG meeting in Southampton (noted above).

### **Evaluation of the Impact of Compute Node Clock Frequency Change**

In November 2022, a configuration change was made such that, by default, jobs would run on compute nodes at 2.0 GHz (previously, the default was 2.25 GHz). The change, documented in [AR2-RFC-150](#), was intended to improve energy efficiency of the service, prompted by favourable evidence for benchmark applications.

Having been in operation for a few months, CSE has begun an evaluation of the impact of the change with the objective of better quantifying the potential energy-efficiency improvements, providing tailored advice to users on how best to run their workflows, and producing recommendations for possible refinements to the configuration.

This work remains on-going and the CSE team hope to produce initial results and recommendations during the coming reporting period.

## ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from January 2023 – March 2023. 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 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	Jan 2023		Feb 2023		Mar 2023		Q1 2023	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	91.0%	2	91.0%	2	91.0%	2	91.0%	2
ARCHER2_CSE_Level2 (MTR)	94.0%	2	97.0%	2	91.0%	2	93.0%	2
ARCHER2_CSE_Level3 (MTR)	100%	1	100%	0.5	100%	1	100%	2.5
ARCHER2_CSE_TA (%)	100%	1	100%	1	100%	1	100%	1
Initial Response to Queries (%)	98.3%	12.5	100%	1	100%	1	100%	2.2
Query User Satisfaction (%)	100%	1	100%	1	97.8%	1	98.5%	1
Training Satisfaction (%)	100%	1	100%	1	100%	1	100%	1
<b>Total</b>		-10.3		-9.5		-11		-28.75

93 query feedback responses were received on query resolution in the Reporting Period. 98.9% 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 January 2023 – March 2023.

### 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.

January 2023					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	57	56	1	3	0.5h
ARCHER2_CSE_Level2	46	45	19	12	0.4h
ARCHER2_CSE_Level3	1	2	5	35	0.1h
ARCHER2_CSE_TA	8	7	1	10	0.2h
February 2023					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	70	71	0	3	0.4h
ARCHER2_CSE_Level2	76	62	33	13	0.3h
ARCHER2_CSE_Level3	0	2	3	50	0.2h
ARCHER2_CSE_TA	4	3	2	12	0.5h
March 2023					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	194	194	0	3	0.3h
ARCHER2_CSE_Level2	75	83	25	15	0.4h
ARCHER2_CSE_Level3	1	2	2	40	0.3h
ARCHER2_CSE_TA	10	9	3	10	0.2h
Q1 2023					
Service level	Assigned	Resolved	Backlog	Correspondence	First Response
ARCHER2_CSE_Level1	321	321	0	3	0.4h
ARCHER2_CSE_Level2	197	190	25	13	0.4h
ARCHER2_CSE_Level3	2	6	2	41	0.2h
ARCHER2_CSE_TA	22	19	3	10	0.3h

## CSE Query Categories

A total of 536 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
<b>ARCHER2_CSE_Level1</b>	Courses	321	59.9%
<b>ARCHER2_CSE_Level2</b>	3rd party software	72	13.4%
	Batch system and queues	23	4.3%
	eCSE applications/calls	19	3.5%
	Courses	14	2.6%
	Software errors	14	2.6%
	Porting, performance and scaling	9	1.7%
	Login, passwords and ssh	8	1.5%
	Software installation	8	1.5%
	Compilers and system software	5	0.9%
	Data transfer	5	0.9%
	Access to services	4	0.7%
	Other: Queries which do not fit within other categories	4	0.7%
	Hardware issue	2	0.4%
	Storage and compute resources	2	0.4%
	SAFE: Queries relating to SAFE	1	0.2%
<b>ARCHER2_CSE_Level3</b>	3rd party software	4	0.7%
	Compilers and system software	1	0.2%
	Software errors	1	0.2%
<b>ARCHER2_CSE_TA</b>	UKRI Grant	13	2.4%
	Pump-priming	5	0.9%
	Fellowship	1	0.2%
<b>Total</b>		<b>536</b>	<b>100.0%</b>

## 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 2023, the CSE service has provided a total of 12.5 days of training, scheduled as follows:

Dates	Course	Days	Attend
18 Jan 2023	Porting OptClim Optimisation system to ARCHER2	0.5	19
25 Jan 2023	OPTIMET: an HPC Code for Modelling Nonlinear Optical Response of Arbitrary Clusters of Nanoparticles on ARCHER2	0.5	7
30-31 Jan 2023	Software Carpentry (Cardiff)	2	15
22-24 Feb 2023	Message Passing programming with MPI (IC, London)	3	21
14 Mar 2023	Introduction to LAMMPS	1	12
22 Mar 2023	The Science behind the Image Competition #1	0.5	11
28-30 Mar 2023	Efficient use of the HPE Cray EX Supercomputer ARCHER2	3	17
30-31 Mar 2023	Data Analysis and Visualisation in Python	2	11

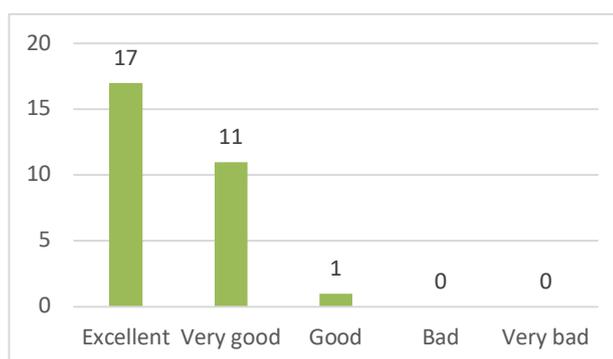
We started the year with two webinars that presented the outcomes of two eCSE projects. Two courses were delivered face-to-face: the Software Carpentry course took place in Cardiff, and the Message Passing programming with MPI course took place at Imperial College, London. The rest of the courses included in the above table took place online. A series of two webinars on the science behind the 2022 ARCHER2 Image and Video Competition were scheduled, one in March and the other one in April. Competition entrants were invited to talk about their work and the science behind their stunning images and videos.

The ARCHER2 training forum meeting was held online at the beginning of March. An invitation was extended to all ARCHER2 users, and all UKRI (EPSRC and NERC) consortia were contacted to send a representative to the meeting. The training programme draft was presented to the audience and future topics were discussed; for example, software build tools such as CMake. Another run of several courses on programming languages like C++ and Fortran was requested by several attendees.

The ARCHER2 training panel meeting took place on Monday, 20 March 2023. Members from inside and outside the UK attended the meeting. A report on the current training year was presented. The candidate version of the ARCHER2 training programme for May 2023 – April 2024 was discussed and approved by all the present members.

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 29 responses, a response rate of 38%.

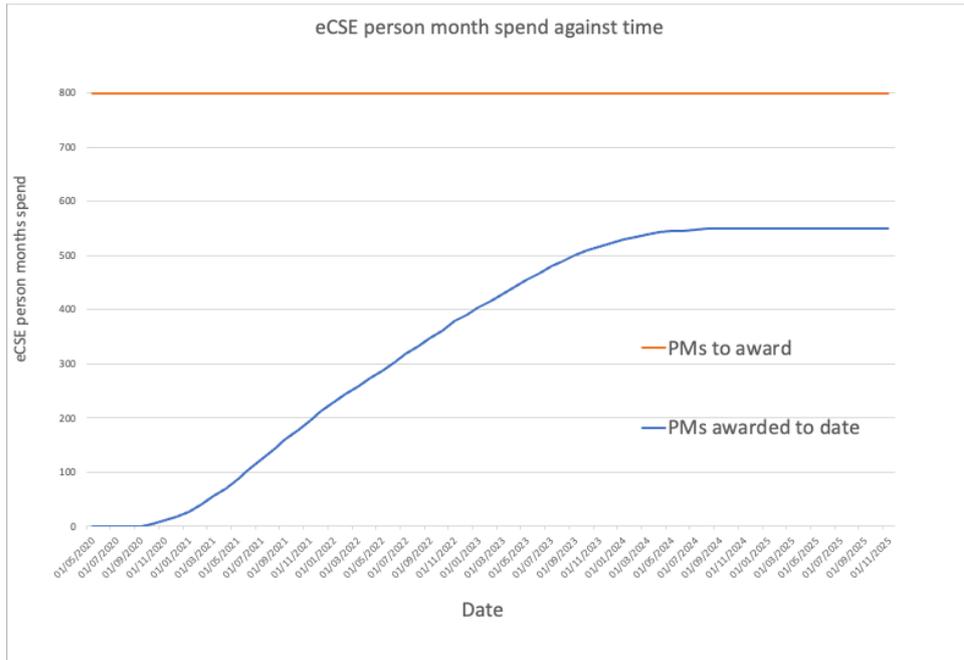


## ARCHER2 Embedded CSE Programme (eCSE)

- eCSE Calls 1-9
  - Call 9 (eCSE09) opened on 6 December 2022. The deadline for submitting documents for technical evaluations was 21 February 2023 and the final deadline for proposal submission was 14 March 2023. The call received 12 technical evaluations followed by 12 proposals requesting a total of 146 person months.
  - The panel meeting to decide which proposals to accept will take place on 13 April 2023.
- For call 1 and from call 5 onwards, only proposals with software within the EPSRC remit have been eligible.
- We plan to open call 10 (eCSE10) on 18 April 2023, closing for technical evaluations on 23 May 2023 with final proposals due on 13 June 2023.
- The recent 18.5 month extension provides an extra 222 PMs of effort bringing the total amount to award to 798 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	11 (8,3)	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)
eCSE09	6/12/22- 14/03/23	12	12(12,0)	146(146,0)	TBD	TBD
<b>Total</b>		<b>125</b>	<b>111(101,10)</b>	<b>1100(879,77)</b>	<b>59(51,8)</b>	<b>549(487,62)</b>

The following graph shows the current person months awarded to eCSE projects to date (blue line) along with the number to be awarded up until the end of the ARCHER2 service including the recent extension (orange line).



## ARCHER2 Community Engagement, Outreach, Collaboration and Impact

### Blogs

2023 has been a busy year for blogs so far. Eight diverse blogs have been written including:

- Rust in HPC, a technical blog discussing how appropriate the Rust programming language is for HPC systems by using a simple computational fluid dynamics (CFD) code to compare between languages
- eCSE Early Career Observer experience, written by one of our early career observers
- The ARCHER2 CSE Team at SuperComputing 22

There have been 407 views of the blogs, with the highest viewing figures achieved by the technical blogs.

### Community and Outreach Activities

The team has been preparing for the **Edinburgh Science Festival (ESF)** and will be offering drop-in sessions at the Royal Museum of Scotland from the 10 – 13 April. New activities have been developed for this event, including a hands-on activity around switches, circuits and building logic gates (AND and OR). A new binary number activity has also been developed with new binary wheel and card activities. New flyers have been developed and new postcards showcasing case studies and the image competition have been prepared. On completion of ESF, the team will focus on the **Big Bang Fair** in Birmingham in June 2023.

A new Wee Archie is under development. Wee Archie has proved very successful for engaging the public in our outreach activities. This new development will continue to allow the science on ARCHER2 to be showcased, but with the opportunity to utilise either CPU or GPU components and with greater monitoring available, including power monitoring.

The **International HPC Summer School** (<https://ss23.ihpcss.org/>) will take place in Atlanta, GA, during 9th–14th July. David Henty, Ludovic Capelli and Weronika Filingier are involved in organising and running the event. There was a record number of applications from UK students (over 30) and 5 of them were selected to attend, along with 9 students from Australia, 9 from Canada, 9 from Japan, 22 from Continental Europe and 27 from the United States.

The ARCHER2 team is also involved in two Birds of a Feather sessions at the **International Supercomputing conference (ISC'23)** in Hamburg, titled:

- *Understanding the Skills and Pathways Behind Research Software Training* – jointly organised with Jeremy Cohen from Imperial Collage London.
- *Another Step Towards the Sustainable HPC Outreach Ecosystem* – the session is a follow up from similar session run last year at SC'22 and this time involves Karina Pesatova from IT4I (Czech Republic), Ann Backhaus from Pawsey (Australia), Bryan Johnston from CHPC (South Africa) and Weronika Filingier from EPCC.

Weronika Filingier was one of the guests on the **Code for Thought** podcast dedicated to RSE training. The episode “Mind the Gap!” was recorded in January and released in March - <https://codeforthought.buzzsprout.com/1326658/12453462-en-mind-the-gap>, with synopsis:

*“There are a lot of excellent training programmes for researchers and RSEs, like the Code Refineries and various Carpentries. But with demand of experienced engineers growing rapidly, we have a gap in*

*training enough RSEs. In this episode I meet with Jeremy Cohen, Radovan Bast, Weronika Filingner and Malvika Sharan to discuss training and what we can do to fill the gap.”*

## Diversity and Inclusivity

The EPCC WHPC Chapter representatives, Eleanor Broadway and Weronika Filingner, are part of the WHPC Workshop committee for the upcoming **ISC'23 conference**. Unfortunately, WHPC did not manage to secure a workshop slot at ISC'23 this year though, working with ISC management, we have been able to develop a strong program of activities, nonetheless.

The WHPC Poster Session will be part of the main ISC program this year. The selected posters will be on display throughout the conference and serve as the focal point for the WHPC Networking Reception on 23 May. More details are available at <https://womeninhpc.org/women-in-hpc-events/whpc-to-isc23>.

WHPC will also host a virtual workshop on 15 May. The event will be free to attend and focus on DEI (Diversity, Equity and Inclusion) issues and early career development. The upside of not running an in-person workshop at ISC is being able to reach more community members by running it online. Going forward, ISC has agreed the WHPC workshop will be one of the invited workshops, so will not need to apply. This will allow more time for planning and fund-raising as well as demonstrating a stronger ISC commitment to addressing the underrepresentation of women in scientific computing.

## Quality Management, Information Security and Business Continuity

After the success of passing our three ISO certifications at the end of 2022, we are in the middle of our usual round of internal audits and improvement activities. We use the ISO methodologies to deliver services, keep a focus on information security, and to prepare for disruptions to service to minimise the likelihood of disruptions happening, and if they do, the user impact. Our external audits happen annually in the autumn, but the cycle of work continues throughout the year. We are currently planning business continuity tests and focusing on how best to prevent cyber security issues such as ransomware.