ARCHER2 CSE Quarterly Report

Oct – Dec 2021

EPCC

The University of Edinburgh

1. Document Information and Version History

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Reviewer(s)	Alan Simpson

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0.1	2021-02-23	Initial draft	Lorna Smith
0.2	2021-12=16	Add training	Juan Rodriguez Herrera
0.3	2021-12-17	Added eCSE	Chris Johnson
0.4	2021-12-21	Centralised component added	George Beckett
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0.6	2022-01-05	Added user feedback, impact and ISO data	Anne Whiting
0.7	2022-01-10	Added ARCHER2 CSE metrics performance report, CSE query statistics and categories	Xu Guo
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ARCHER 2 Quarterly Report

This section of the report covers the period October 2021 – December 2021 for the ARCHER2 service.

2. ARCHER2 Executive Summary

- During this period the service reached a significant milestone, with the full ARCHER2 system being made available to the user community. The CSE team carried out comprehensive testing in advance of this, updated the documentation, and fielded a high volume of queries.
- We delivered a webinar to introduce the ARCHER2 full system, this had a record attendance of 156 people.
- The CSE team contributed to the Witnessed Acceptance Trial in mid-November and early-life support during the stability period.
- Finally the team has supported the user community on both the 23-cabinet and 4-cabinet systems, until the 4-cabinet system was removed from service in January.
- CSE has joined a collaboration with HPE to evaluate a containerised version of the Cray Programming Environment, which will potentially give ARCHER2 users much greater flexibility to develop and test software and workflows for the service.
- Three virtual tutorials and six courses have been delivered in this period, constituting a total of 10.5 training days. The ARCHER2 full system has been used successfully for several courses and virtual tutorials.
- The fifth eCSE call closed for technical evaluations on 5 Oct 2021 receiving 10 proposals for technical evaluation, with the call itself closing on 26 Oct 2021 receiving 9 full proposals. At the panel meeting on 23 Nov 2021, 5 of these proposals were selected for funding, awarding 46 PMs in total.
- The fifth eCSE call opened alongside an Early Career eCSE Observers call. These observer calls give researchers in the early stages of their careers an opportunity to attend a panel meeting giving them an insight into the grant/proposal selection processes. 14 applicants were accepted with 4 of them attending the recent panel meeting.
- We have run the popular ARCHER2 image and video competition and 3 very worthy winners were selected for the three categories, best image, best video and winning best career researcher entries.
- The entries from the image competition from 2020 and 2021, plus pictures of the ARCHER2 installation and ARCHER2 team, have been combined to produce the ARCHER2 calendar, which showcases the science on ARCHER2. Copies have been sent to members of the community.
- Work has commenced to prepare for ISO 22301 certification. This is a business continuity standard which will help to ensure we are further prepared with resilient services and robust plans to be able to restore them should major incidents ensure.
- A total of 142 pieces of query feedback have been received for the CSE service from a total of 537 queries handled. All feedback was rated good and above, with the majority excellent.
- A donation of £1 per user feedback response has been made to our selected charity, Save the Children. This quarter a total donation of £289 has been made, with £142 from CSE Query feedback.
- CSE staff wrote an article promoting HPC-related career opportunities in MyFuture magazine, which aims to disseminate opportunities for underrepresented and minority communities in the UK.
- Weronika Filinger helped deliver a full programme of student HPC activities at the Supercomputing 2021 conference.
- With a relaxation of Covid-19 restrictions during autumn, we saw several scientific-community meetings organised. The CSE team promoted and represented the ARCHER2 service at a number of these meetings.

- The ARCHER2 service had a table (together with the Cirrus service) at the CIUK exhibition in December 2022. This allowed the service to be presented to the user and HPC communities, showcasing the science being carried out.

3. ARCHER2 Forward Look

- Charging will be implemented on the full system from January. That will then be the first period that has the full system available to users with appropriate peer reviewed budgets in place. As such CSE anticipates working with the user community to maximise their utilisation on this significant resource. For example by supporting communities to scale to previously unavailable core counts.
- A full programme of courses is planned, benefitting from the full system. Due to COVID restrictions, training has so far all been online, which has led to some unexpected advantages to the user community (as well as some disadvantages). In the future, we plan to offer a mixture of online and in-person training. During this next quarter, we plan to survey the user community to understand their preferred mechanism for course delivery, to determine the optimal balance between online and in person training.
- Having welcomed the first 4 of the 14 early career observers to the recent eCSE panel meeting, we are looking forward to welcoming 10 over the next few upcoming panel meetings. We will be looking for feedback from attendees on the value of the opportunity and if/how this scheme can be improved.
- Benefits realisation metrics have been implemented in SAFE, allowing reporting of information related to projects such as industrial and international collaborators and subject area. These metrics help provide evidence of the value of the ARCHER2 service. Now that charging has been introduced on the full system, metric data can be obtained, and this will be reviewed during the coming months to ensure the correct data is being collected.

4. ARCHER2 Centralised CSE Team

CSE work during the period focused on the final preparations for bringing the main system into service, in October and November, followed by early-life support for users during the stability trial. In particular, the CSE team contributed to final validation of the main system, in early November, and participated in the ARCHER2 Witnessed Acceptance Tests, held at the ACF during 15th—17th November.

The online user documentation was significantly updated to address differences between the 4-cabinet and the main system, including the move to a new version of the Cray Shasta software and a move to the LMod module system (from the TCL module system). Furthermore, the portfolio of supported software was tested and updated to work with the main system.

The CSE team continued to engage with the user community, including the following community focused activities:

- Michael Bareford presented at the CompBioMed seminar in October (https://www.compbiomed.eu/compbiomed-e-seminar-18/).
- Andrew Turner gave a presentation about the ARCHER2 service at the RSE HPC Champions Meeting on 26th October.
- Michael Bareford also presented an introduction to ARCHER2 for a week-long Unified Model training course in November.
- William Lucas represented the ARCHER2 service at the UKCTRF annual meeting in December (https://www.ukctrf.com/index.php/upcoming-events-2021/).
- Juan Herrera participated in the Computing Insight UK meeting, during 9th—10th December, staffing the EPCC booth, which featured lots of publicity and information for the ARCHER2 service.
- Andy Turner also participated in the HPC-SIG Meeting on 7th December and the RSE Leaders Network Meeting on 15th December.
- Lorna Smith presented at the BOF "Words Matter! Promoting Inclusion through Language in Advanced Research Computing" at SC21, Wednesday 17th November 2021.

CSI Projects

HPE CPE Containers Customer Evaluation Programme

During the period, the CSE team joined the HPE CPE Containers Customer Evaluation Programme, which is investigating the scope and benefits of providing a containerised version of the Cray EX Programming Environment, which researchers could use to develop and test applications and workflows on local resources before moving onto ARCHER2. The investigation is in its early stages, though we hope to make some initial conclusions early in 2022.

Benchmarking and optimising the performance of centrally supported codes NAMD and NEMO

Eleanor Broadway and Xu Guo have completed their investigations into the benchmarking, optimisation and tuning of NAMD and NEMO applications, based on the ARCHER2 4-cabinet system.

For both NAMD and NEMO, it is common for users to run fewer processes than physical CPU cores, due to memory limitations. For NAMD, this has been shown to potentially lead to poorer performance, though the issue can be mitigated by running shared-memory threading on the free cores. For NEMO, little performance loss occurs, even in the absence of threading, so the user can employ the free cores to run the XIOS IO servers. The team found that scalability was also improved in NAMD by having some cores entirely dedicated to communication. In all cases it is important to match the distribution of processes and threads to the NUMA architecture of the nodes.

Our advice to users on the optimisation and tuning of NAMD and NEMO has been summarised within the PRACE T7.5 final deliverable and a best practice guide will be added to the ARCHER2 documentation in due course.

Beyond the optimisations on the ARCHER2 4-cabinet system, within PRACE T7.5, the team will continue with further performance tests for comparison based on the PRACE Tier-0 system, Joliot-Curie, which has a similar processor architecture to ARCHER2 but a different network (Infiniband). We would expect to see the same qualitative effects in terms of performance, but the optimal parameter choices could be different.

Porting and Optimisating CP2K for the ARCHER2 Main System

Holly Judge continued to tune the supported deployment of the CP2K application suite. Changes were made to the QM/MM module, to tune to the specific configuration of the main system.

Further work, to port the QM/MM module to the grid API is in progress, alongside an evaluation of the software on the AMD Accelerator Cloud, which supports GPU offloading of calculations via the HIP framework. The outputs of these activities will be fed into the ARCHER2 service in the coming periods.

5. ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from October 2021 until end of December 2021.

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. *Initial MTR applicable to OY1: Service Threshold: >4.4 WD; Operating Service Level: >1.4 WD, ≤2.4 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. *Initial MTR applicable to OY1: Service Threshold: >27 Working Days (WD); Operating Service Level: >12 WD, ≤17 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. *Initial MTR applicable to OY1: Service Threshold: >59 Working Days (WD); Operating Service Level: >29 WD, ≤39 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 OY1: 8 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%.*

On 22 November, the full (23-cabinet) system came into Service alongside the 4-cabinet system. UKRI requested that SLAs should apply to the full system from this date. The following table, therefore, includes figures based on the ARCHER2 4 Cabinet service from 1 October to 22 November 2021 and figures based on the ARCHER2 full system service from 22 November to 31 December 2021.

Metric	October 2021		November 2021		December 2021		Q4 2021	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR) (4c)	0.1WD	-2	0.1WD	-2		-2	0.1WD	-6
ARCHER2_CSE_Level1 (MTR) (full)			0.1WD		0.1WD		0.1WD	
ARCHER2_CSE_Level2 (MTR) (4c)	0.4WD	-2	0.1WD	-2		-2	0.3WD	-6
ARCHER2_CSE_Level2 (MTR) (full)			0.2WD		0.3WD		0.3WD	
ARCHER2_CSE_Level3 (MTR) (4c)	29WD	0	6WD	-2		-2	18WD	-4
ARCHER2_CSE_Level3 (MTR) (full)			-		8WD		8WD	
ARCHER2_CSE_TA (%) (4c)	100%	-1	100%	-1		-1	100%	-3
ARCHER2_CSE_TA (%) (full)			100%		100%		100%	
Initial Response to Queries (%)	99.6%	-0.25	99.3%	-0.25	99.2%	-0.25	99.4%	-0.75
Query User Satisfaction (%)	100%	-2	100%	-2	100%	-2	100%	-6
Training Satisfaction (%)	94%	-0.25	100%	-1	94%	-0.25	95%	-1.5
Total		-7.5		-10.25		-9.5		-27.25

126 query feedback responses were received on query resolution in the Reporting Period. 100% of responses had a score of “Good”, “Very Good” or “Excellent”.

6. ARCHER2 CSE Queries

This section provides details on ARCHER2 CSE queries during the Reporting Periods from October 2021 until end of December 2021.

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.

The following table includes figures based on the ARCHER2 4 Cabinet service from 1 October to 22 November 2021 and figures based on the ARCHER2 full system service from 22 November to 31 December 2021.

October 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1 (4c)	156	155	2	3	0.7 hrs
ARCHER2_CSE_Level2 (4c)	86	82	21	11	0.4 hrs
ARCHER2_CSE_Level3 (4c)	0	1	4	39	0.4 hrs
ARCHER2_CSE_TA (4c)	9	7	3	15	0.8 hrs
November 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1 (4c)	34	36	0	4	0.5 hrs
ARCHER2_CSE_Level1 (full)	5	6	0	4	0.6 hrs
ARCHER2_CSE_Level2 (4c)	43	46	18	12	0.4 hrs
ARCHER2_CSE_Level2 (full)	66	37	31	9	0.4 hrs
ARCHER2_CSE_Level3 (4c)	1	1	4	38	0.2 hrs
ARCHER2_CSE_Level3 (full)	2	0	2	-	-
ARCHER2_CSE_TA (4c)	15	9	9	12	0.5 hrs
ARCHER2_CSE_TA (full)	1	4	1	10	0.9 hrs
December 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1 (full)	46	46	0	3	0.4 hrs
ARCHER2_CSE_Level2 (full)	67	71	27	14	0.4 hrs
ARCHER2_CSE_Level3 (full)	2	1	3	65	0.2 hrs
ARCHER2_CSE_TA (full)	4	4	1	13	1.6 hrs

Q4 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Correspondence**	**First Response**
ARCHER2_CSE_Level1 (4c)	190	191	0	4	0.6 hrs
ARCHER2_CSE_Level1 (full)	51	52	0	3	0.4 hrs
ARCHER2_CSE_Level2 (4c)	129	128	18	11	0.4 hrs
ARCHER2_CSE_Level2 (full)	133	108	27	12	0.4 hrs
ARCHER2_CSE_Level3 (4c)	1	2	4	39	0.3 hrs
ARCHER2_CSE_Level3 (full)	4	1	3	65	0.2 hrs
ARCHER2_CSE_TA (4c)	24	16	9	13	0.6 hrs
ARCHER2_CSE_TA (full)	5	8	1	12	1.2 hrs

CSE Query Categories

A total of 506 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 (4c)	Number resolved (full)	% Queries
ARCHER2_CSE_Level1	Courses	191	52	48.0%
ARCHER2_CSE_Level2	3rd Party Software	30	50	15.8%
	Login, passwords and ssh	22	10	6.3%
	Batch system and queues	12	13	4.9%
	Compilers and system software	13	12	4.9%
	eCSE Applications/Calls	19	1	4.0%
	Access to HPC	12	2	2.8%
	Performance and scaling	3	6	1.8%
	Porting	3	5	1.6%
	Data Transfer	4	3	1.4%
	User programs	4	-	0.8%
	Courses	2	1	0.6%
	Node Failure	1	2	0.6%
	Network	2	-	0.4%
	Queue Time	1	1	0.4%
	Disk, tapes, resources	-	1	0.2%
	SAFE	-	1	0.2%
ARCHER2_CSE_Level3	3rd Party Software	2	-	0.4%

	Compilers and system software	-	1	0.2%
ARCHER2_CSE_TA	Access to HPC	6	5	2.2%
	Pump priming	5	3	1.6%
	UKRI Grant	5	-	1.0%
Total		337	169	100%

7. ARCHER2 Training

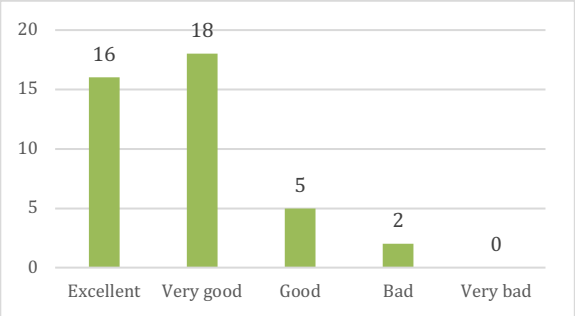
As part of ARCHER2, the service has been developing and delivering an online training programme for the ARCHER2 community. During the last quarter of 2021, the CSE service has provided a total of 10.5 days of online training, scheduled as follows:

Dates	Course	Days	Attend
5, 8 Oct 2021	Advanced OpenMP	2	12
11-12 Oct 2021	Introduction to CP2K	1	23
20 Oct 2021	Parallel I/O on ARCHER2	0.5	35
28 Oct 2021	Understanding Package Performance on ARCHER2	1	15
17 Nov 2021	Introduction to the full ARCHER2 system	0.5	156
29-30 Nov 2021	ARCHER2 for software package users	2	16
1 Dec 2021	ARCHER2 user drop-in session	0.5	5
2 Dec 2021	ARCHER2 for software package users	1	6
6-7 Dec 2021	Data Carpentry	2	34

We have offered several courses and virtual tutorials where the ARCHER2 full system has been the main topiuc. The virtual webinar where the ARCHER2 full system was introduced beat the attendance record with 156 attendees.

The Data Carpentry course was organised in collaboration with Heriot-Watt University (HWU). The course proved to be very popular among HWU post-graduate students. Several experienced helpers from HWU also took part in the course, making the course more informative as well as enjoyable.

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 4.17, i.e., better than “Very Good”. Users provided 41 responses, a response rate of 39%. As usual, the feedback responses have been carefully reviewed and actions such as updating the course description of some courses will be performed when the next run takes place.



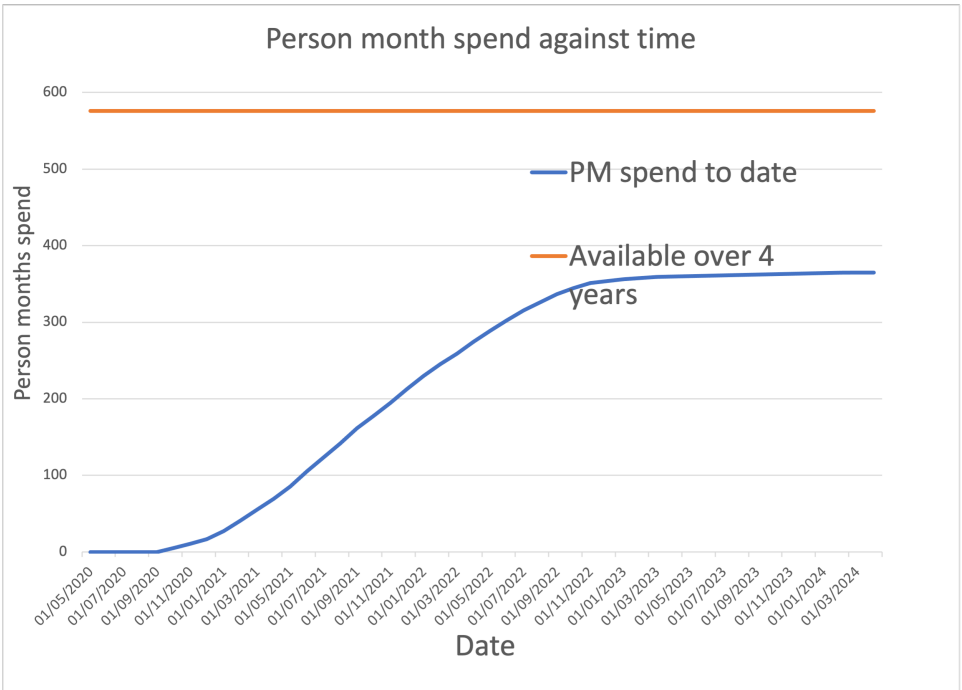
8. ARCHER2 Embedded CSE Programme (eCSE)

eCSE calls 1-5

- From the first 5 calls, 365 PMs have been awarded across 40 projects. These are detailed in the table below.
- From call 5 onwards, only proposals with software within the EPSRC remit have been eligible.

eCSE call	Call dates	# Technical evaluations received	# Proposals received (EPSRC,NERC)	# PMs 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)	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)
Total		**76**	**72 (62,10)**	**672 (595,87)**	**40 (32,8)**	**365 (303,62)**

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).



9. ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Community Engagement and Impact

SC21

Weronika Filinger (CSE) chaired the **student programming at SC21 conference** in November (https://sc21.supercomputing.org/). The role had started during the previous conference (SC20, in November 2020) with the creation of the committee (8 members - from Australia, Germany, South Africa, UK and USA), which over the subsequent year prepared a programme of online sessions that ran throughout SC21.

Student programming consists of a number of sessions prepared for students participating in other SC Student Programs (e.g., Student Volunteers, competitions, HPC immersion) and other student attendees. Traditionally, the sessions an only on the Sunday and Monday, so as not to clash with other SC activities. Due to the on-going global situation, this year, SC21 was run in a hybrid format, which allowed the committee to do many things that would not be possible otherwise. Moving the program online made it possible to expand it – in terms of content, the number and diversity of the invited speakers, and the reach of the programme.

MyFuture Magazine

The article "*Find your place in High Performance Computing*", written by Neelofer Banglawala and Weronika Filinger, was published in the MyFuture Magazine's Education and Careers Guide for 2021/2022. The magazine is the UK's leading diversity and inclusion, education and careers multi-media platform, helping employees recruit diverse talent and promote equality, diversity and inclusion. The article, also featuring Craig Morris, is available to read online at https://issuu.com/bls-media/docs/myfuture_issue_4_21-22 (pages 68-70).

CHPC'21

Ben Morse was invited as a panellist to participate in the *"Online Education: Surprises and Insights"* Birds of a Feather session, during the CHPC 21 conference. The session discussed some of the challenges in moving to an online education platform. Three speakers from three different regions talked about their experiences of implementing online programmes, what surprises they experienced along the way, and what insights they could share with others trying to move to an online education model.

Outreach Activities and Events

After a long period of a lack of face-to-face events due to the COVID pandemic, the Computing Insight UK (CIUK) meeting was held in person during 9th—10th December. EPCC had a stand/booth at the event which showcased ARCHER2 (and the Cirrus Service). This was a welcome return to face-to-face events and we were able to feature information about the ARCHER2 service, to promote and disseminate the service to the UK community.

Quality Management and Information Security

After the success of our re-certification external audit for ISO 27001, the information security standard, and surveillance audit for ISO 9001, quality service delivery, work continues with the round of internal auditing and improvement activity to ensure that we maintain and improve the services we deliver to our users. We have started work on the preparation needed for ISO 22301, the business continuity and disaster recovery standard to ensure that we apply best practice in this area.