ARCHER2 Quarterly Report

January – March 2021

EPCC

The University of Edinburgh

1. Document Information and Version History

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Author(s):	Lorna Smith, Juan Rodriguez Herrera, Chris Johnson, Xu Guo, Anne Whiting, George Beckett
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This section of the report covers the period Jan 2021, Feb 2021 and March 2021 for the ARCHER2 service.

2. ARCHER2 Executive Summary

- During the period, CSE effort has been focused on early-life support for the ARCHER2 4-cabinet service, which opened in early January. CSE has handled a predictably large number of in-depth queries and has focused on providing the best possible response to these queries. This has allowed users to utilise the service quickly, and utilisation has indeed been very high.
- We have been monitoring queue utilisation closely and have put in place a series of changes to help support users during this busy period. While wait times are still longer than would be ideal, this does demonstrate a clear appetite from the user community for the full 23 cabinet system.
- The CSE team has also been preparing for early access to the 16-cabinet system when it arrives during the next quarter. A clear plan of work has been developed for the three week access period, with a view to ensuring the user environment is tested, documented and fit for purpose for the user community.
- While attending user meetings and visiting consortia in person has not been possible with COVID, the CSE team has endeavoured to engage with users in other ways. We have continued to contribute to the ARCHER2 webinar series, participated in online consortium meetings from the Materials Chemistry Consortium and the UK Consortium on Turbulent Reacting Flows, and worked to ensure consortium contacts support consortia appropriately.
- The first ARCHER2 User Training Forum took place in March. The Forum is composed of members of all the UKRI scientific consortia and provides input into the design and delivery of the training programme. The training programme draft for the upcoming year was discussed and additional courses added based on feedback.
- A new online self-service course on OpenMP was published in February. Self-service courses are valuable as they allow people to access training when it suits them, making courses accessible to a wider range of people.
- Three members of the ARCHER2 team wrote, editorial material for the Spring 2021 edition of BAME Magazine, for the magazine's education and careers guide. Neelofer Banglawala, Craig Morris, and Weronika Filinger showcased opportunities in HPC and the scientific community, in a four-page feature article.
- As part of the celebration of Women's History Month (March 2021), the Supercomputing Conference, in collaboration with Women In HPC, published a series of blog articles titled "Meet Six Trailblazing Women in HPC". This included EPCC's Linda Dewar.
- 10 blog articles have been published this quarter with highlights being the video documenting the end of the ARCHER service and the video of the installation of the majority of the ARCHER2 cabinets at the ACF.
- Three eCSE calls have successfully been issued during the first year of ARCHER2, providing an important opportunity for ARCHER2 users and RSEs to access funding to support software development. The programme continues to be popular, with the third call receiving 14 proposals; these are presently under review.
- Evidence from the first two eCSE calls suggests that the use of award letters and associated terms and conditions is working well for all parties involved.
- To encourage users to provide feedback, we make a donation of £1 per response to a chosen charity. This quarter a donation of £374 has been made to Save the Children.

3. ARCHER2 Forward Look

- During this next period we anticipate gaining access to the 16-cabinet system for a short 3-week period. During this time the team will test, port, document and prepare for users gaining access to the full 23-cabinet system. The aim is to ensure users are able to make a quick and seamless transfer to the 23-cabinet system when available.
- Having monitored and investigated the queue structure on the 4-cabinet system, we plan to engage with the user community on our proposed queue structure for the full system. The aim is to ensure this structure is fit for purpose for the community.
- Having handled a significant number of in-depth queries during Q1 of 2021, we are confident that problem identification processes are working well. Monitoring, identifying and solving common problems across multiple queries will continue to be key as we move to the larger system and we will continue to engage pro-actively with Cray HPE to solve these problems.
- Following on from the ARCHER2 User Training Forum held in March, the ARCHER2 Training Panel will meet in April to review and approve this training programme for the upcoming year.
- The first year of training under ARCHER2 is now almost complete. COVID 19 has led to a very different look and feel to training, however our online training offering has proved very popular and has provided some advantages such as enhanced flexibility. The team will look to review the delivery of these courses, understanding feedback and identifying room for improvement. The aim is to continue to provide high quality training that is able to adapt to changing working environments for our users.
- In April, HPE Cray will deliver an advanced course that will provide attendees with the knowledge required to understand the most optimal way to port, execute and optimize applications for ARCHER2.
- From the 4th eCSE call onwards, the eCSE will allow shorter projects from 1-3 PMs, in addition to those awarded 3-12 PMs. This bridges the gap between in-depth queries and existing eCSE effort (requiring more than 3 PMs of effort).

4. ARCHER2 Centralised CSE Team

During the period, CSE effort has been focused on early-life support for the ARCHER2 4-cabinet service, which opened in early January. With a significant increase in the number of users on the 4-cabinet system, CSE has handled a predictably large number of in-depth queries (mostly, CSE Level 2) as project teams familiarise themselves with the capabilities of the new service and migrated their existing research campaigns from ARCHER.

The CSE team worked closely with the hardware vendor to identify and resolve a small number of problems, not identified during early-access, which impacted certain use cases. Most notably, several key applications were affected, when used at research scale, by memory leaks in the underlying Cray Programming Environment. At the time of writing, a new version of the Programming Environment is being deployed by HPE Cray staff to address these issues. The CSE team also helped HPE Cray staff to diagnose problems with clean-up of resources at the end of CASTEP jobs and with out-of-memory errors for users undertaking code-profiling work.

The CSE team has also continued to contribute to the ARCHER2 webinar series, with sessions on containerised workflows and on using software-management features of GitHub to promote better research software engineering, being featured during the period.

Several HEC held their annual meetings during the period and CSE consortium contacts participated in those. Holly Judge presented an overview of ARCHER2 and her work on benchmarking materials-chemistry codes at the Materials Chemistry Consortium meeting on 29th January. Further, William Lucas contributed to the UK Consortium on Turbulent Reacting Flows that ran their workshop on 30th and 31st March, receiving feedback on the new service and fielding comments about queueing time charging.

CSI Projects

The CSE team continued to progress several, early-life service-improvement projects, as follows:

- Work on the X-Alt software logging tool has been put on hold temporarily, as we await the logging infrastructure on ARCHER2 to be finalised – something that we expect to be done for the full service. In the meantime, we have investigated options to extract a subset of the information we could get from X-Alt, from the (Slurm) scheduling system's built-in database.
- Adrian Jackson completed an evaluation of the ARCHER2 inter-node communication system; to confirm that changes to the configuration of the high-speed network (HSN), required to address a potential security vulnerability, did not adversely affect application performance. The benchmarks provided good coverage of the performance of the HSN, across a range of typical use cases, and confirmed the configuration changes would not affect performance. The benchmarks are more generally useful and will be used as part of readiness evaluation of the full system when CSE have access in April.
- With support from the PRACE initiative, Eleanor Broadway and Xu Guo have been benchmarking and optimising the popular molecular-dynamics model, NAMD. The main purpose of this project is to provide advice and best practice to ARCHER2 users on the optimal running conditions for NAMD as well as providing general advice on optimising the performance of different compilers and libraries available on ARCHER2. The current focus is on benchmarking, profiling and optimising NAMD based on the ARCHER2 4-cabinet system. Further work will be carried out on the full ARCHER2 system once it is available, as well as one of the PRACE Tier-0 system with similar architecture, through which we will also be able to advise users on moving between ARCHER2 and Tier-0 systems. The project should be completed by the end of 2021.

5. ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods from Jan 2021 until end of March 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%.*

Metric	Jan 2021		Feb 2021		March 2021		Q1 2021	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	0.1 WD	-2	0.1 WD	-2	0.1 WD	-2	0.1 WD	-6
ARCHER2_CSE_Level2 (MTR)	0.4 WD	-2	0.4 WD	-2	0.4 WD	-2	0.4 WD	-6
ARCHER2_CSE_Level3 (MTR)	43 WD	1	17 WD	-2	25 WD	-0.5	25 WD	-1.5
ARCHER2_CSE_TA (%)	100%	-1	100%	-1	100%	-1	100%	-3
Initial Response to Queries (%)	100%	-1	100%	-1	99.5%	-0.25	99.8%	-2.25
Query User Satisfaction (%)	97.4%	-2	100%	-2	100%	-2	99.4%	-6
Training Satisfaction (%)	100%	-1	100%	-1	100%	-1	100%	-3
Total		-8		-11		-8.75		-27.75

154 query feedback responses were received on query resolution in the Reporting Period. 99.4% of responses had a score of "Good", "Very Good" or "Excellent".

In Jan 2021, one ARCHER2_CSE_Level3 query took 43 WD. This was a complex code query which ultimately became a mini project and has now been resolved.

6. ARCHER2 CSE Queries

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

CSE Query Statistics

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER2 CSE Service Contract.

- **No. of Assigned:** The number of CSE queries assigned to the Contractor within each query resolution category in the Reporting Period.
- **No. of 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
- **Avg No. of Correspondence:** The average number of pieces of correspondence generated for CSE queries in each query resolution category.
- **Avg Time for First Responses:** The average time taken for the Contractor to first respond to the Originator of the CSE query.

A total of 662 queries were resolved by the ARCHER2 CSE service in the Reporting Period.

Jan 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average no. of Correspondence**	**Average Time for First Response**
ARCHER2_CSE_Level1	81	79	2	4	0.4 hrs
ARCHER2_CSE_Level2	106	62	48	13	0.4 hrs
ARCHER2_CSE_Level3	9	1	16	7	0.1 hrs
ARCHER2_CSE_TA	4	3	3	13	0.4 hrs
Feb 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average no. of Correspondence**	**Average Time for First Response**
ARCHER2_CSE_Level1	161	155	8	4	0.6 hrs
ARCHER2_CSE_Level2	139	140	47	13	0.4 hrs
ARCHER2_CSE_Level3	5	9	12	30	0.4 hrs
ARCHER2_CSE_TA	9	11	1	13	0.3 hrs
March 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average no. of Correspondence**	**Average Time for First Response**
ARCHER2_CSE_Level1	44	52	0	4	0.4 hrs
ARCHER2_CSE_Level2	115	131	31	13	0.3 hrs
ARCHER2_CSE_Level3	1	5	8	26	0.1 hrs
ARCHER2_CSE_TA	16	14	3	11	0.5 hrs
Q1 2021					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average no. of Correspondence**	**Average Time for First Response**
ARCHER2_CSE_Level1	286	286	0	4	0.5 hrs
ARCHER2_CSE_Level2	360	333	31	13	0.4 hrs
ARCHER2_CSE_Level3	15	15	8	27	0.3 hrs
ARCHER2_CSE_TA	29	28	3	12	0.5 hrs

CSE Query Categories

Resolved CSE queries in the Reporting Period fell into the following categories:

Service level	Category	Number resolved	% Queries
ARCHER2_CSE_Level1	Courses	286	43.2%
ARCHER2_CSE_Level2	3rd Party Software	128	19.3%
	Batch system and queues	53	8.0%
	Compilers and system software	46	6.9%
	eCSE Applications/Calls	21	3.2%
	User programs	19	2.9%
	Porting	18	2.7%
	QueueTime	8	1.2%
	Performance and scaling	8	1.2%
	Access to HPC	8	1.2%
	Login, passwords and ssh	7	1.1%
	Disk, tapes, resources	6	0.9%
	Data Transfer	4	0.6%
	Other	3	0.5%
	Hardware Problem	1	0.2%
	Node Failure	1	0.2%
	Network	1	0.2%
	Courses	1	0.2%
ARCHER2_CSE_TA	UKRI Grant	19	2.9%
	Non-UKRI Grant	4	0.6%
	Pump priming	3	0.5%
	Access to HPC	2	0.3%
ARCHER2_CSE_Level3	3rd Party Software	13	2.0%
	User programs	1	0.2%
	Batch system and queues	1	0.2%
Total		662	100.0%

7. ARCHER2 Training

As part of ARCHER2, the service has been developing and delivering an online a training programme for the ARCHER2 community. During the first quarter of 2021, the CSE service has provided a total of 18.5 days of online training, scheduled as follows:

Dates	Course	Days	Attend
12 Jan 2021	ARCHER2 for Software Package Users	1	25
13 Jan 2021	Patterns for Research Software Management using GitHub	0.5	54
14-15 Jan 2021	Introduction to ARCHER2 for Software Developers	2	22
18-21 Jan 2021	Software Carpentry	2	19
25 Jan 2021	Understanding Package Performance (*)	1	9
28-29 Jan 2021	Performance Optimisation on AMD EPYC (*)	2	23
3 Feb 2021	eCSE ARCHER2 Webinar	0.5	15
22-23 Feb 2021	HPC Carpentry	2	20
10 Mar 2021	Exploding, Forming and Disentangling Stars with HPC	0.5	25
10-11 Mar 2021	Computational Thermal Hydraulics using Code_Saturne (*)	1	16
17, 22, 24 Mar 2021	Message-passing Programming with MPI	3	24
29-30 Mar 2021	Introduction to ARCHER2 for Software Developers	2	7
30 Mar 2021	Containers in HPC	0.5	25
31 Mar 2021	Quantum Computing Without A Quantum Computer	0.5	29
Total		18.5	284

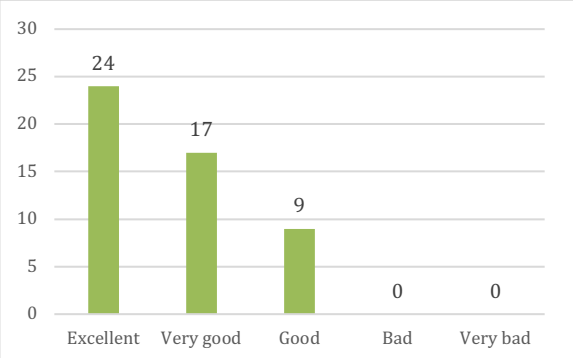
The above table lists a total of five virtual tutorials and nine courses, three of these courses are new (marked with an asterisk).

Additionally, we collaborated on a five-day introductory course delivered by the University of Manchester. The course covered shell scripting, version control and task automation. We introduced the researchers to HPC environments using the ARCHER2 HPC facility; more than 20 attendees had access to the machine. While there was potentially a mismatch between the levels of the overall course and the ARCHER2 material, these forms of collaboration can be a positive way for the ARCHER2 training team to interact with the user community and will be considered in the future.

A new online self-service course on OpenMP was published in February. Self-service courses provide value as they allow people to access training when it suits them. Registrations are always open. More than 20 people have already registered.

In March, the first ARCHER2 User Training Forum took place. The Forum is composed of members of all the UKRI scientific consortia. The mission is to provide ongoing input into the design and delivery of the training programme. The training programme draft for the upcoming year was discussed and some courses were added based on feedback received from the Forum.

On the feedback for online courses, attendees rated the course on a scale of 1-5 (“Very Bad”, “Bad”, “Good”, “Very Good” and “Excellent”). The average feedback using this metric was 4.3, i.e., better than “Very Good”. Users provided 50 responses, a response rate of 31%.



8. ARCHER2 The Embedded CSE Programme (eCSE)

As part of ARCHER2, the CSE service will deliver an eCSE programme to provide embedded CSE support across the UK. The service will deliver an average of 12 FTEs over its lifetime. Over the first 4 years of the ARCHER2 service this will provide 576 PMs of which 185 have been awarded from the first two calls as detailed below. Projects awarded effort receive an award letter and PIs are asked to confirm they confirm with our Terms and Conditions document. Evidence from the first two calls suggests this process is working very well and is less time consuming than the model used under ARCHER.

The 1st ARCHER2 eCSE call

- The first eCSE call opened for proposals on the 19th May 2020 and closed on the 7th Jul 2020. This received 25 proposals from a broad range of subject areas within the EPSRC remit, with PIs from 15 different UK Institutions. Overall a total of 235 PMs of effort was requested from 13 different UK institutions.
- From this call 13 projects were awarded a total of 132 PMs overall. Most projects have started with one project delayed due to COVID; this will start during the next quarter.

The 2nd ARCHER2 eCSE call

- The second eCSE call opened on the 8th Sep 2020 and closed on the 27th Oct 2020 initially receiving 13 technical evaluations of which 12 became full proposals from 11 different UK institutions. Overall a total of 107 PMs of effort were requested. This call was open to codes from both the EPSRC and NERC remits.
- From this call 7 projects were awarded a total of 53 PMs overall.
- Projects have either started or will start during the next quarter.

The 3rd ARCHER eCSE call

- The third eCSE call opened on the 8th Dec 2020 and closed on the 16th Mar 2021, 4 weeks later than planned due to the potential effects of lockdown on applicants. The call initially received 15 technical evaluations of which 14 became full proposals from 11 different UK institutions. Overall a total of 136 PMs of effort were requested from technical staff at 12 different UK institutions. As for the previous call, this was open to codes from both the EPSRC and NERC remits.
- The panel meeting to decide on which projects to award will take place on the 8th April 2021.

The 4th ARCHER eCSE call

- The 4th call is planned to open on 20 Apr 2021, closing for technical evaluations on the 28th May and for full proposals on the 8th Jun 2021.
- The ARCHER2 service will provide a full spectrum of support from in-depth queries (which take a few days or weeks to resolve) up to full eCSE projects which presently run from 3-12 PMs. To cover the gap for work requiring 1-3 PMs, from the 4th call onwards, eCSE calls will allow proposals to request effort from 1-12 PMs. This introduces shorter projects requiring less detail in the proposal form – all of which will be described in the application guidance.

Future calls

- Calls will be issued three times per year with a regular timetable based on similar dates to those for the calls described above.

9. ARCHER2 Community Engagement, Outreach, Collaboration and Impact

Reflecting CSE's commitment to advocating and increasing inclusivity and diversity within HPC community, the team members have engaged in the below activities.

- The ACM SIGHPC Education Chapter created a new committee with the aim of setting up an educational award, and Weronika Filinger – in her role of a co-chair of the outreach committee – has been asked to join the initiative. The new committee put together a proposal for a new ACM award for Outstanding Contribution to Computational Science Education. One of the important criteria of the award - to be given to individuals for their work on a specific educational project or initiative – is the ability to engage, serve and retain a diverse community of participants. The award is currently under consideration by the ACM awards committee. If accepted, it will be awarded annually at the Supercomputing Conference in November.
- Three members of the ARCHER2 team wrote, under the banner of Women In HPC, editorial material for the Spring 2021 edition of BAME Magazine, for the magazine's education and careers guide. BAME Magazine aims to raise the aspiration levels of young people from BAME backgrounds looking for career choice guidance and information on further education and apprenticeship opportunities. Neelofer Banglawala, Craig Morris, and Weronika Filinger showcased opportunities in HPC and the scientific community, in a four-page feature article. The magazine is due to be published in April 2021.
- The ISC21 organisers invited the BoFs accepted to ISC20 (and subsequently cancelled) to present at this year's virtual conference. Weronika Filinger is the leader of the "Scalable and Effective Online HPC Education and Training" session, which will focus on possibilities of online learning in the context of HPC education and training. One of the advantages of online education is that it can be more scalable, accessible and inclusive than traditional in-person opportunities, and thus can easily open a path towards greater diversity in our community.
- The planning for SC21 has accelerated after the virtual kick-off meeting held in February. Weronika Filinger as the chair of the Student Programming put together a diverse committee with members from Europe, North America, Africa, Asia and Oceania. The committee has started preparing the conference program for students. The planning work requires close cooperation with other SC committees, including the Inclusivity (especially, its Early Careers sub-committee) and Communications committees.
- As part of the celebration of Women's History Month (March 2021), the Supercomputing Conference, in collaboration with Women In HPC, published a series of blog articles titled "Meet Six Trailblazing Women in HPC", with the intention to inspire others to pursue a career in HPC. EPCC's Linda Dewar was one of the six trailblazers featured, describing her role to coordinate the installation, commissioning and testing of ARCHER2.

10 blog articles have been published this quarter with highlights being the video documenting the end of the ARCHER service and the video of the installation of the majority of the ARCHER2 cabinets at the ACF. We plan to continue to publish regular blogs on all aspects of the service, technical and otherwise. We also hope to feature blog articles from the user community on the exciting science being created on ARCHER2 once the full service goes live, and from UKRI on their role in the service.

Users submitting queries to the service desk with a SAFE account have been asked for feedback on the handling of their query. A donation of £1 per user feedback response has been made to our selected charity, Save the Children. This quarter a donation of £374 has been made.