ARCHER CSE Service Quarterly Report

Quarter 4 2016

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1. Executive Summary

This report covers the period: 1 October 2016 to 31 December 2016 inclusive.

- Centralised CSE Team:
  - We have produced a best practice guide for parallel I/O on ARCHER that will help users get the best performance out of the ARCHER file systems: http://www.archer.ac.uk/documentation/best-practice-guide/io.php
  - The parallel I/O studies have led to us proposing that default striping be changed to improve responsiveness and performance for most users.
  - In consultation with major user groups we have completed a paper proposing an updated set of ARCHER benchmarks.
  - We have worked with SP and Cray to expand the performance metrics automatically gathered on the system to include energy and memory usage. This data is now imported into SAFE and can be queried by users to understand better the resources they are using.
- Training:
  - We delivered 13.5 days (250 student-days) of face-to-face training in the quarter at 4 different locations, with an average feedback score better than "very good".
  - A one-day hands-on course "Using Knights Landing Manycore Processors on ARCHER" was successfully run for the first time, and will form the basis of an extended 2-day course to be held early in 2017.
  - A new KNL-specific version of the ARCHER Driving Test has been launched.
  - Based on feedback from ARCHER Champions, we have also launched a version of the ARCHER driving test targeted at package users (i.e. non-developers).
  - The plan for the 2017 training programme was approved by the ARCHER training panel.
- ARCHER Outreach Project:
  - The ARCHER Image competition was very successful, with 43 images received. The ARCHER Calendar was produced, printed and posted before Christmas.
  - WHPC held a full day workshop and hosted two BoFs at SC16 and was recognised once again in the annual HPCWire Readers' and Editors' Choice Awards, receiving the Readers' Choice: Workforce Diversity Leadership Award; the Editors' Choice: Workforce Diversity Leadership Award and the Readers' Choice: Outstanding Leadership in HPC, for Toni Collis, Director of WHPC.
  - We demonstrated Wee Archie at the IET Engineering the Future Festival to an estimated 300 school children. The event was organised by the Institute of Engineering and Technology in London on the 6th October.
  - Wee Archlet, a smaller build your own Raspberry Pi cluster has been developed and will be tested in Q1 2017.
  - We held an Outreach BOF at SC16. Prior to this, a Q&A style article was published by HPCWire, which raised the profile of the event.
  - One new case study is online and 25 eCSE project highlights are now available. See: http://www.archer.ac.uk/casestudies/ and http://www.archer.ac.uk/community/eCSE/
- eCSE:
  - Of 72 projects from the first 9 eCSE calls, 66 have now started and 47 have already completed; the remaining 6 projects are due to start within the next quarter. Of those completed, 40 final reports have been received.
  - The eCSE09 call received 19 proposals; 5 of these were selected for funding at the Panel meeting on 13 December, awarding a total of 62 person months. Following on from feedback from the Panel, the proposal form was streamlined for this call.
  - A call for Early Career Researcher Panel Observers was opened on 16 December 2016 and will close 17 January 2017. Successful candidates will be chosen to attend Panel meetings during 2017.

2. Collaborations and Outputs Summary

- Presentations:
  - Andy Turner and Adrian Jackson, Parallel Models and Scaling, Keynote Talk, EuroMPI, Sep 2016, Edinburgh UK
  - Nick Brown, MONC - highly scalable cloud modelling on the latest supercomputers, SC16, Nov 2016, Salt Lake City, USA
  - Rupert Nash, HemeWeb: Simple, reproducible blood flow simulation in the cloud using containers, RCUK Cloud Workshop, Nov 2016, London, UK
  - Adrian Jackson and David Henty, ARCHER HPC Training, Third SC Workshop on Best Practices for HPC Training, Nov 2016, SC16, Salt Lake City, USA https://sites.google.com/a/lbl.gov/hpc-training-best-practices/workshops/sc16
  - Adrian Jackson, Parallel Performance: Moving MPI applications to the next level, Intel HPC Developers conference, Nov 2016, Salt Lake City, USA http://www.intel.com/content/www/us/en/events/hpcdevcon/technical-sessions.html
  - Adrian Jackson, NEXTGenIO: Moving I/O into the memory system by Adrian Jackson, Nov 2016, Exascale I/O: Challenges, Innovations and Solution, SC16, Salt Lake City, USA
  - Nick Brown, MONC - highly scalable cloud modelling on the latest supercomputers, Computing Insight UK, Dec 2016, Manchester, UK
- Meetings:
  - Andy Turner, EPSRC Software Workshop, Oct 2016, London
- Papers:
  - Y.A.G. Fosado, D. Michieletto, J. Allan, C.A. Brackley, O. Henrich, D. Marenduzzo, A Single Nucleotide Resolution Model for Large-Scale Simulation of Double Stranded DNA, Soft Matter 12, 9458-9470 (2016).
  - O. Wiese, D. Marenduzzo, O. Henrich, Microfluidic Flow of Cholesteric Liquid Crystals, Soft Matter 12, 9223-9237 (2016).
- Posters:
  - Neelofer Banglawala, Bespoke bone modelling with VOX-FE, SC16, Nov 2016, Salt Lake City, USA
  - Adrian Jackson, Mario Antonioletti, Vadim Biktashev, Irina Biktasheva,, Sanjay Kharche and Tomas Stary , BeatBox — HPC Simulation Environment for Biophysically and Anatomically Realistic Cardiac Electrophysiology, SC16, Nov 2016, Salt Lake City, USA

3. Forward Look

- KNL System:
  - We will use the new ARCHER benchmarks (and other suitable benchmarks) to compare the performance of the KNL system to the main ARCHER system and publish a public report with the findings to help the user community better understand the opportunities and challenges associated with KNL technology.
- Application Landscape:
  - Using the new memory and energy usage metrics that are being pulled into the SAFE database, we will analyse the data report on energy and memory usage on the service to provide insight into usage. This will be useful information for optimising the current system configuration and for any future system procurements.
- Parallel I/O:
  - An update to the parallel I/O white paper comparing performance on ARCHER with other systems has been written and is currently in review. This will be released and publicised shortly.
- Training:
  - We will analyse feedback from the recent training impact survey and circulate the report.
  - An extended 2-day version of the recent KNL course will be developed.
  - Based on user feedback from recent courses, we plan to:
    - continue to run interactive online quizzes during courses using the Socrative system as these have received positive feedback;
    - consider the possibility of developing new courses on software testing and high-level software architecture (feedback received from "Practical Software Development");
    - look at revising the material from the new course "Writing Scalable Parallel Applications" to introduce a motivating example program (from CFD) at the outset, returning to it throughout the course.
- ARCHER Outreach Project:
  - EPSRC have a display at the American Association for the Advancement of Science meeting in Boston in February. Wee Archie has been invited to form part of this display and Nick Brown will be attending the meeting to demonstrate the system.
  - We will add new interviews to the "Faces of HPC" page to increase the number of interviews while maintaining a broad spectrum of individuals.
  - In early 2017, ARCHER will run an Introduction to Message Passing Programming course that will be aimed at the Women in HPC community.
  - Planning for WHPC events in 2017 is already underway with submissions for workshops at ISC 2017 and SC17, and planning for the third annual WHPC UK event in the first half of 2017.
  - Planning for the 3rd ARCHER Champions Workshop is underway. This will be held in conjunction with HPC-SIG in Leeds on 9th and 10th February, and will focus on interactions with the new Tier 2 centres.
  - We have a booth at the Big Bang Fair in March 2017, and effort in Q1 2017 will focus on preparing for this event.
  - Further case studies in the pipeline include a biomolecular simulation project. We also plan to develop case studies with a selection of image competition entries.
- eCSE:
  - We are planning ahead for the remaining 3 eCSE calls to balance the award of the remaining person months so as to provide maximum benefit to ARCHER users given the remaining time left on the ARCHER service.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: October 2016, November 2016 and December 2016.

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

CSE Query Metrics

- **QE1:** The percentage of all queries notified to the Contractor by the Help Desk in a Quarter that the Contractor responds to, and agrees a work plan with, the relevant End User within 3 working hours of receiving the notification from the Help Desk. *Service Threshold: 97%; Operating Service Level: 98%.*
- **QE2:** The percentage of all queries notified by the Help Desk to the Contractor that have been satisfactorily resolved or otherwise completed by the Contractor within a 4-month period from the date it was first notified to the Contractor. *Service Threshold: 80%; Operating Service Level: 90%.*
- **TA1:** The percentage of all technical assessments of software proposals provided to the Contractor by the Help Desk in any Service Period that are successfully completed by the Contractor within 10 days of the technical assessment being provided to the Contractor by the Help Desk. *Service Threshold: 85%; Operating Service Level: 90%.*
- **FB1:** The percentage of End User satisfaction surveys for CSE queries carried out in accordance with the Performance Monitoring System by the Contractor showing the level of End User satisfaction to be "satisfactory", "good" or "excellent". *Service Threshold: 30%; Operating Service Level: 50%.*

Period	Oct-16		Nov-16		Dec-16		Q4 2016	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
QE1	100%	-2	100%	-2	100%	-2	100%	-6
QE2	100%	-2	100%	-2	100%	-2	100%	-6
TA1	100%	-1	100%	-1	92%	-1	100%	-3
FB1	100%	-2	100%	-2	100%	-2	100%	-6
Total		-7		-7		-7		-21

Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level

Training Metrics

- **FB2:** The percentage of all training satisfaction surveys carried out in accordance with the Performance Monitoring System by the Contractor) in each Quarter that are rated "good", "very good" or "excellent". *Service Threshold: 70%; Operating Service Level: 80%.*

Period	Oct-16		Nov-16		Dec-16		Q4 2016	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
FB2	100%	-1	100%	-1	100%	-1	100%	-3
Total		-1		-1		-1		-3

Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level

Service Credits

Period	Oct-16	Nov-16	Dec-16
Total Service Points	-8	-8	-8

5. CSE Queries

Queries Resolved in Reporting Period

Metric Descriptions

In-Depth	All technical queries passed to ARCHER CSE team
Course Registration	Requests for registration on ARCHER training courses or enquiries about registration
Technical Assessment: <Category>	Request for Technical Assessments of applications for ARCHER time
eCSE Application	Queries relating to eCSE applications

A total of 269 queries were resolved by the CSE service in the reporting period.

Metric	Oct-16	Nov-16	Dec-16	Total	% Total
Course Registration	94	92	6	192	71.4%
In-Depth	8	9	16	33	12.3%
eCSE Application	4	3	11	18	6.7%
Technical Assessment: Grant	1	2	10	13	4.8%
Course Enquiry	0	1	5	6	2.2%
Technical Assessment: Instant	1	2	2	5	1.9%
Technical Assessment: HEC	1	0	0	1	0.4%
Technical Assessment: RAP	0	0	1	1	0.4%

8 query feedback responses were received on In-depth queries in the reporting period. This represents a 28% return rate for feedback forms. All 8 responses registered a score of "Excellent".

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	25	75.8%
User programs	4	12.1%
Compilers and system software	2	6.1%
Batch system and queues	2	6.1%

In-Depth Query Highlights

A small number of In-Depth queries have been selected to illustrate the work of the centralised CSE team over the reporting period.

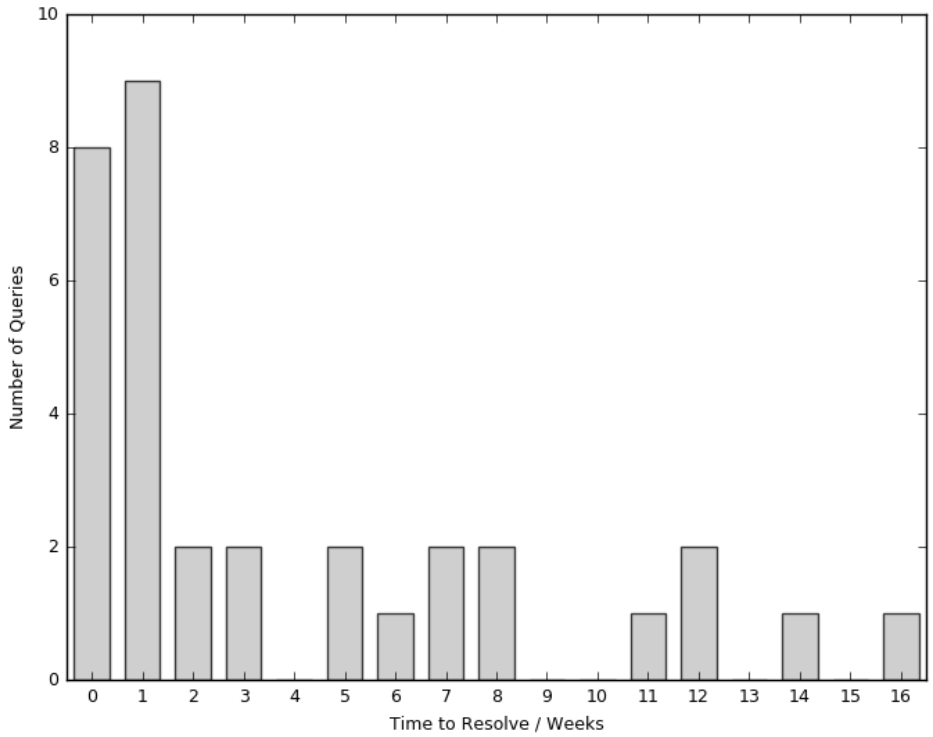
Q770825: FHI-Aims
A user was seeing issues with the materials science application FHI-AIMS freezing at random points when running their calculations. The CSE team isolated the problem to a subtle issue with floating point precision differences between different parallel processes in the application, which was leading to the non-deterministic behaviour. The user was advised on best practice for setting the multiple convergence tolerances in the application so that such issues could be avoided, and is now able to run their calculations successfully.

Q781145: performance variability
User reported that they see large performance variations with identical runs of their simulation using their own application (from ~20h to ~40h time to solution) and wondered how they might improve this situation. The CSE service took a deep dive into the performance of the application to understand the performance variation. The analysis was very complex as there were three separate aspects that were introducing variability: Lustre metadata server performance; Lustre bandwidth contention; and interconnect contention. We provided an updated routine to improve

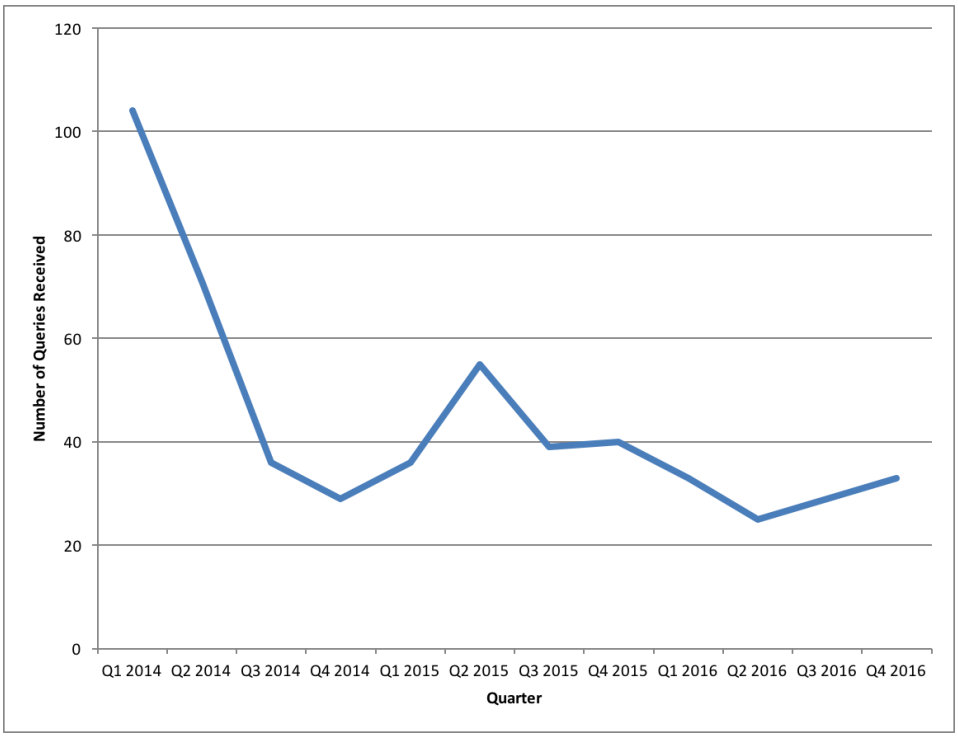
the performance with respect to the Lustre metadata server (the original version was issuing many needless open/close operations) and provided data to quantify the variation from the other two sources so that the user could build enough contingency into their jobs. Advice was provided on how the user may change their application to potentially decrease interconnect contention going forwards. Throughout the query, the CSE team kept the user aware of how we were making progress so that they understood the process of analysing the performance and would be able to put it into practice themselves in the future when developing their software.

In-Depth Query Analysis

The histogram below shows the time to resolution for In-Depth queries in the current reporting period. The median resolution time during this period is 1 weeks (median resolution time since 1 Jan 2014 is 2 weeks).

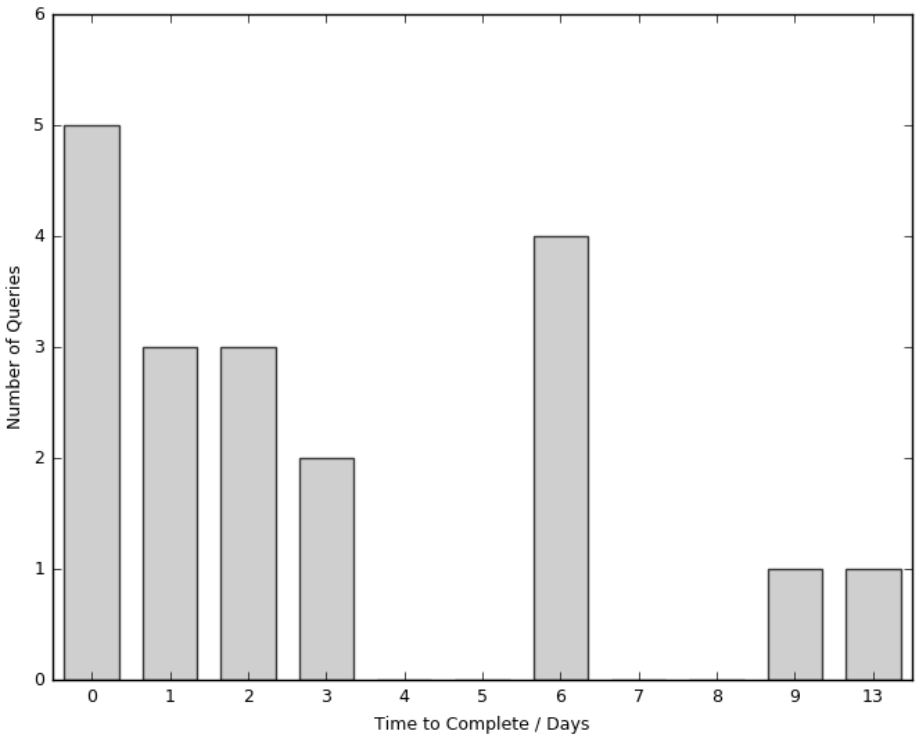


Plot of numbers of In Depth queries received per quarter:

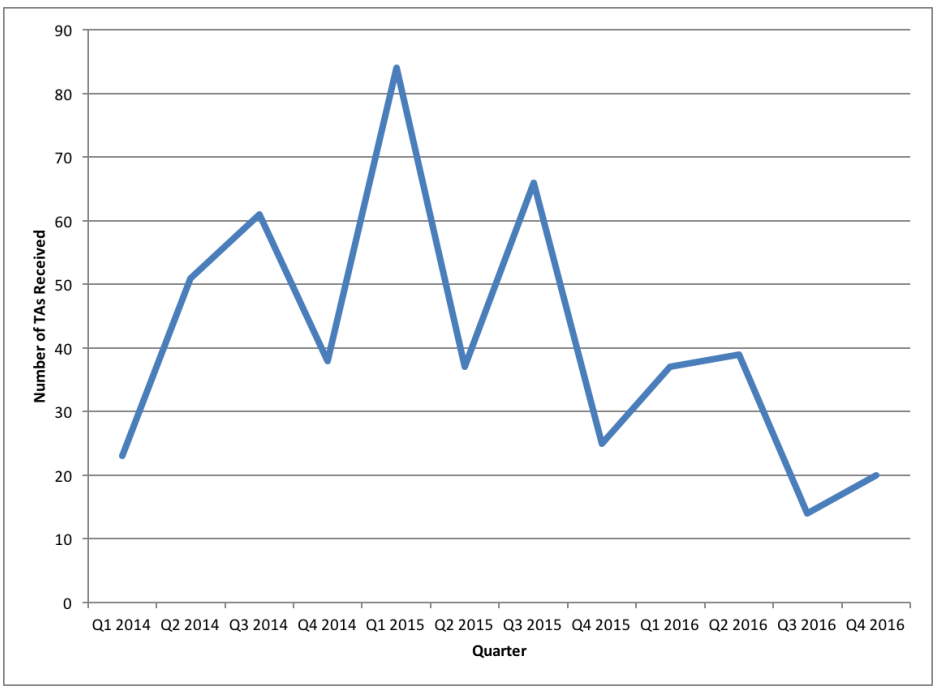


Technical Assessment Analysis

A histogram of the time to completion for Technical Assessments (see below) reveals that the median completion time for this quarter was 2 days (median completion time since 1 Jan 2014 is 3 days).



Plot of numbers of Technical Assessments received per quarter:



6. Centralised CSE Team: Strategic Priorities Progress

In collaboration with user groups and the other Service partners, the CSE service identified several priority areas to invest technical effort from the centralised CSE team. This section summarises progress in the reporting period in these areas.

Parallel I/O Performance

We have updated the *benchio* parallel I/O application (https://github.com/EPCCed/benchio) to implement a *file-per-process* scheme for parallel I/O to compliment the single-shared-file scheme that was already available.

This new functionality has been used to benchmark the file-per-process scheme for parallel I/O and compare the performance to the single shared file scheme. The results from this analysis have formed the basis of the ARCHER parallel I/O best practice guide (http://www.archer.ac.uk/documentation/best-practice-guide/io.php) and the soon to be released white paper comparing parallel I/O across different systems.

This work has also led to a recommendation that the ARCHER service changes the default Lustre stripe value from 4 to 1. This change will lead to improved interactive responsiveness and consistency of performance for all users with little impact on performance. Users who perform large-scale, shared-file parallel I/O already need to explicitly set the stripe count to -1 (maximum striping) to obtain useful performance so this change should not impact them unduly.

Future work in this activity will look at:

- Application specific I/O performance using monitoring data collected automatically from the service;
- Statistical performance data to better understand the variability of performance and the origins of any variability.

Understanding the ARCHER Application Landscape

Work has focussed on two areas:

- Automatic collection of extended application data from ARCHER into SAFE;
- Completion of the updated ARCHER benchmark proposal paper and collection of the application benchmark cases.

SAFE has been extended to pull data from the Cray ALPS scheduler logs and from the Cray Resource Usage Reporting (RUR) tool, and to link the data provided by these sources to the existing job records in the database.

- Cray ALPS logs provide information on the application being used in each job (e.g. VASP, Gromacs) and detailed information on how the compute resources are used within the job (number of processes per node, number of sub-jobs within the main job).
- RUR records provide information on the amount of memory used by each job and the energy usage by each job.

By integrating this data into SAFE, we gain the ability to analyse the data in ways broken down by any property that SAFE knows about. For example, we could analyse application usage by project or research area, or we could analyse energy usage by application type.

We have completed the benchmark proposal paper in consultation with major user groups and have started to gather the benchmark cases. So far, we have gathered cases for 3 out of the 5 application benchmarks and are in discussion with user groups around the other 2 applications.

Future work includes analysing the new data in SAFE and running the application benchmark cases on ARCHER and ARCHER KNL.

7. Training

In the reporting period, the CSE Service has provided a total of 13.5 days (250 student-days) of face-to-face training across four different locations and 2.5 days of interactive online tutorials (average attendance 15 per tutorial).

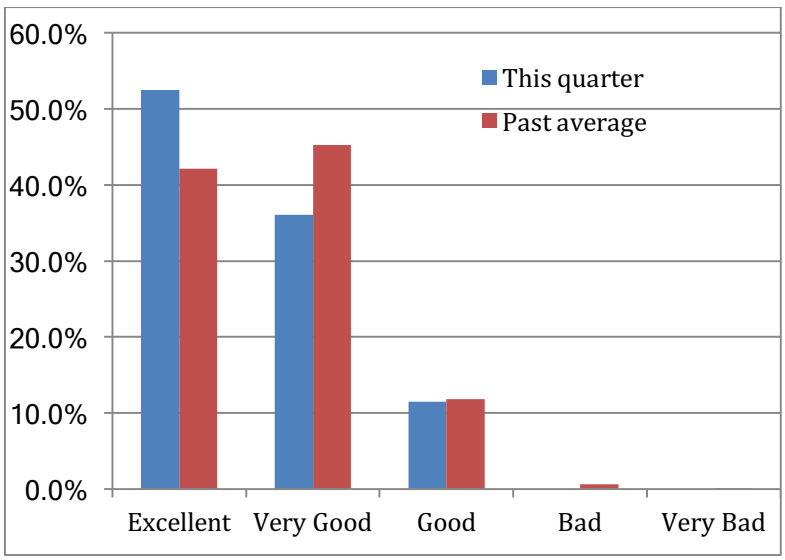
Month	Dates	Course	Location	Days	Attendees
Oct 2016	11-12	GPU Programming with CUDA	London	1.5	20
	12	Using KNL on ARCHER	Online	0.5	
	19	Biological systems in LAMMPS	Online	0.5	
Nov 2016	1	Using KNL on ARCHER	Edinburgh	1	15
	2-3	Data Carpentry	Edinburgh	2	22
	9	Large-Eddy Simulation	Online	0.5	
	23	CP2K: Recent performance improvements	Online	0.5	
	28-29	Single-Node Performance Optimisation	Manchester	2	13
	30	Adjoint ocean modelling	Online	0.5	
	30 Nov – 2 Dec	Message-Passing Programming with MPI	London	3	21
	30 Nov – 1 Dec	Hands-On Introduction to HPC	Newcastle	2	26
Dec 2016	12-13	Writing Scalable Parallel Applications using MPI	Manchester	2	10

On the feedback for face-to-face 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 4.4, i.e. better than "Very Good". Users provided 61 feedback forms, a response rate of 45%.

At the end of their 12-month project, Driving Test users are asked to complete a survey about their experiences. We recently received very positive feedback from two users who were preparing for a full application for ARCHER time:

"ARCHER provided every tool I expected from an HPC cluster. I think the scheme worked well, you should provide the same quality in the future. My experience with ARCHER is very good. The HPC team is very helpful and I think the ARCHER development environment is user-friendly."

"Entirely successful. I was able to get my applications running on ARCHER with minimum fuss, at least in part because the Cray/SLURM/intel/gnu environment is well designed (and common)."



20 days of face-to-face training are planned for the first quarter of 2017, plus 1.5 days of online training.

Month	Dates	Course	Location	Days	Attendees
Jan 2017	11	Modern Fortran	Online	0.5	
	31 Jan – 2 Feb	Cray Optimization Workshop: ARCHER and Knights Landing	Bristol	3	
Feb 2017	8	Parallel I/O	Online	0.5	
	8-10	Performance Analysis Workshop	Southampton	3	
	TBC	Introduction to Scientific Programming with Python	London	2	
	TBC	Message-Passing Programming with MPI	London	3	
Mar 2017	8	TBC	Online	0.5	
	TBC	Efficient Parallel IO on ARCHER	Durham	2	
	TBC	Programming the Manycore Knights Landing Processor	London	2	
	TBC	Single-Sided Communications	Warwick	2	
	29-31	Shared-Memory Programming with OpenMP	Southampton	3	

8. Outreach Project

Diversity

Diversity in HPC (www.hpc-diversity.ac.uk)

We continue to populate the "Faces of HPC" page, which aims to celebrate diversity in the HPC community. Currently we have 12 interviews and 13 historical biographies available online. Over the next year we will continue to add interviews to these pages to increase the number of biographies while maintaining representation from a broad spectrum of individuals.

Women in HPC

WHPC held a full day workshop and hosted two BoFs at SC16. Both were well attended, with the workshop being the first full day event we have held and the most successful workshop to date. Of 49 feedback forms that were collected for the workshop, respondents gave an average score of 4.5 out of a maximum of 5 for their experience at the workshop. The sessions included: methods for improving diversity in the workplace; early career development including posters for early career women; 'Skills to thrive in the HPC community'; as well as case studies on tackling unconscious bias, stereotype threat and implicit bias.

WHPC has been recognised once again in the annual HPCWire Readers' and Editors' Choice Awards, receiving the following honours:

- Readers' Choice: Workforce Diversity Leadership Award
- Editors' Choice: Workforce Diversity Leadership Award
- Readers' Choice: Outstanding Leadership in HPC, for Toni Collis, Director of WHPC

In early 2017, ARCHER will be running an Introduction to Message Passing Programming course that will be aimed at the Women in the HPC community. In addition, planning for WHPC events in 2017 is already underway with submissions for workshops at ISC 2017 and SC17 due in early February 2017, and planning for the third annual WHPC UK event in the first half of 2017.

User Engagement and Skills Development

Planning for the 3rd ARCHER Champions Workshop is underway. This will be held in conjunction with HPC-SIG in Leeds on 9th and 10th February. It will focus on integration with the new Tier 2 centres and registration is already open.

The ARCHER champions web site contains a list of the current ARCHER champions: http://www.archer.ac.uk/community/champions/names/

Finally, we are currently planning the next Hands-on Porting and Optimisation Workshop for Q2 2017.

Outreach

The last quarter has seen significant activity around Outreach, with the development of Wee Archlet, the building of a second Wee Archie, working with a local school to develop the teachers pack, development of the CFD wing demo, demonstrating wee ARCHIE at the IET Engineering the Future Festival in London, and holding an outreach BOF at SC16.

Wee Archlet: a smaller build your own Raspberry Pi cluster has been developed. Instructions have been written and will be tested internally in Jan 2017 with an expectation of release to external testers in Feb/March 2017.

Teacher's pack and school material: work has progressed on the school materials, focusing on the basics of computers and moving into the use of computers in science. We have been working closely with a local Primary school to help develop these materials, working with two upper primary classes. This will continue in 2017 with topics including programming linked to science experiments, supercomputer uses and concepts.

A second "Wee Archie": has been built to meet demand. A Wing (CFD) Simulation demonstration is under development. This has been tested at a public event and future work will focus on providing a more intuitive feedback mechanism for users to see their wing performance. The demonstration framework, which the Wing Simulation is the first to use, will be updated to reflect feedback and observed performance issues during Q1 2017.

*SC16 Outreach BOF: w*e ran a BoF at Supercomputing entitled "HPC Outreach: Promoting supercomputing to the next generation". The aim of this was to bring together people who are currently doing, or would like to do, outreach and then to share ideas, success stories and materials. Prior to the BoF a Q&A style article was published by HPCWire

(https://www.hpcwire.com/2016/11/09/bof-boost-supercomputing-outreach-skills/)

which raised the profile of the event. The BoF was led by EPCC together with representatives from PRACE, XSEDE, Southern California Earthquake centre, and Georgia Institute of Technology.

IET Engineering the Future Festival: organised by the Institute of Engineering and Technology, this was held in London on the 6th October with an aim of celebrating the achievements of the global engineering community. We demonstrated Wee Archie, using the new CFD Wing demo, to an estimated 300 schoolchildren.

Impact Material

Two new case studies have been developed. One is currently online:

- One new case study online: *Understanding changes in the Ganges river delta under climate change*
  https://www.archer.ac.uk/casestudies/ARCHER_casestudy_Bangladesh.pdf

The other is complete and will be published on the web site and publicised in Jan 2017:

- *A new frontier for material science: Designing Nanocomposites in the virtual laboratory*

Leaflets and postcards were created for all the case studies and disseminated via the EPCC booth at SC16.

25 eCSE highlights (from completed eCSE projects) are now on the website. See: http://www.archer.ac.uk/community/eCSE/. In addition, consortium highlights are available for a selection of consortia, for example for UKCP and UKCTRD. See: https://www.archer.ac.uk/community/consortia/ukcp/ and http://www.archer.ac.uk/community/consortia/ukctrf/.

The ARCHER Image competition was very successful, with 43 images received. The overall winner was Dr Peter Falkingham, Liverpool John Moores University with his "The birth of a footprint" image. The ARCHER Calendar was produced, printed and posted before Christmas.

In 2017 we will continue to develop new case studies to ensure this remains fresh and representative of the science and impact on ARCHER. Further case studies in the pipeline include a biomolecular simulation project. We also plan to develop case studies with a selection of image competition entries.

Summary Report for ARCHER Champions Workshop 1

Josephine Beech-Brandt
April 2016

The first ARCHER Champions Workshop took place in Edinburgh in March and was a lunchtime-lunchtime one day meeting, including an evening meal.

There were 23 attendees and 5 bursaries were awarded to cover reasonable travel and accommodation costs.

As this was the first workshop a general overview of several aspects of ARCHER was covered and also discussions regarding the objectives for Champions.

Topics Covered:

- Welcome and Objectives for ARCHER Champions
- Overview of ARCHER as a National resource and how it fits within the National HPC Infrastructure
- Migrating to ARCHER: Common Issues Encountered
- Tours of ARCHER
- ARCHER Training : Locations, Topics
- SAFE Demonstration
- Outreach Session
- The eCSE Programme
- ARCHER Support Structure : How we assist users and access routes for ARCHER
- Discussion : ARCHER Champions, where next?

Outcomes:

- Feedback from attendees was very positive
- Mailing list and ARCHER website list of Champions were created
- Slides were all placed on the Champions website
- Opportunity to link with RSE Fellows and also key HPC-SIG personnel
- Information gathered from the tour and equipment
- Created and strengthened links with EPSRC, local and regional HPC centres, RSE fellows
- Would like future events to be colocated if possible with HPC-SIG/RSE events
- Would like more discussion and interactive sessions if possible
- Next Champions event to be held in Oxford at OeRC in September with focus on the eCSE activity

Summary Report for ARCHER Champions Workshop 2

Josephine Beech-Brandt
October 2016

The second ARCHER Champions Workshop took place in Oxford (thanks to OeRC) in September and was a lunchtime-lunchtime one day meeting, including an evening meal.

There were 25 attendees, 10 of which had attended the first Champions workshop, and 3 bursaries were awarded to cover reasonable travel and accommodation costs.

There was an in-depth look at the eCSE activity, a session on the newly announced KNL system, and updates from other sites. Time for discussion sessions was included.

Topics Covered:

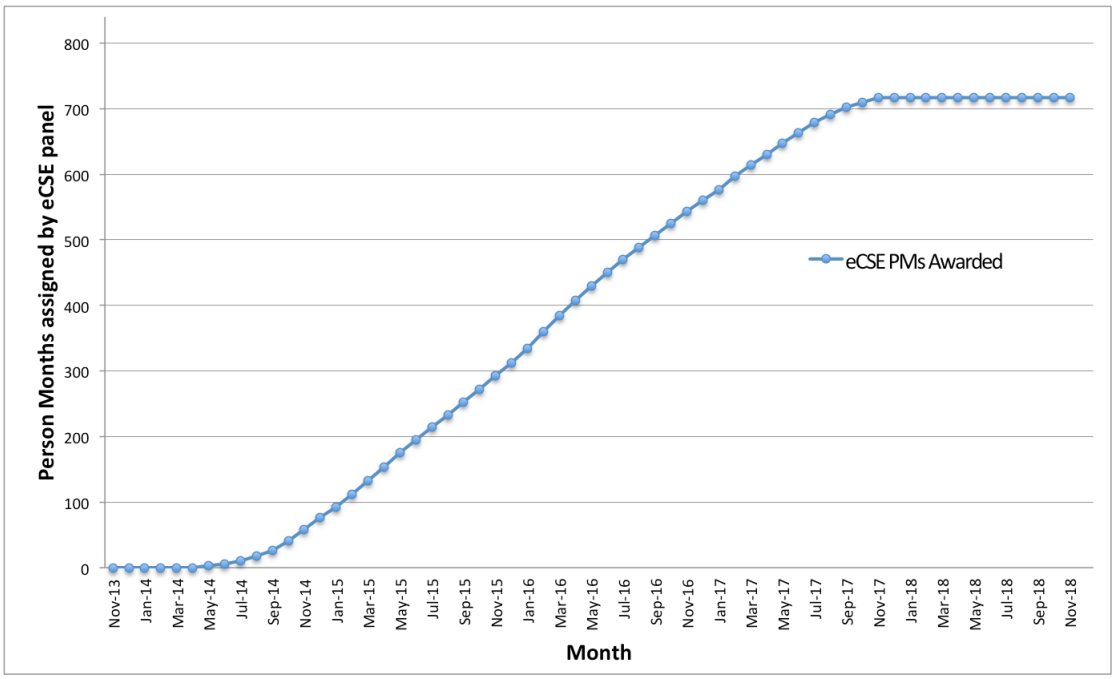
- HPC Service Provision for the UK
- GPU Provision
- KNL on ARCHER
- ARCHER SAFE Updates and Developments
- Outreach activities using Wee Archie as a focus
- Getting started on ARCHER
- More in-depth look at the eCSE activity

Outcomes:

- Good number of attendees with 10 repeat attendees (expand if possible in future)
- Feedback from the attendees (overall very positive)
- Discussion sessions went well (try to include more in future, one each half session)
- Champions making use of ARCHER Champions Project time
- Good to get more external contributors and plan to increase for Champions 3
- Look to monitor what Champions are doing
- Opportunity to engage with users and Tier-2 sites
- Slides were all placed on the Champions website
- Slack channel within RSE space was created
- Use of Champions email for Training and Tier 2 for local dissemination
- Next Champions event with HPC-SIG in Leeds in February with focus on Tier 2 and Training

9. Embedded CSE (eCSE)

Overview of eCSE Effort



- The eCSE person months awarded up to and including the 9th eCSE call are shown in blue
- At least 840 person months will be awarded by the end of the project (14 FTEs for 5 years)
- 732 person months have been awarded so far over 72 supported eCSE projects

eCSE Call 1 – Call 9

eCSE call	No. proposals	No. projects awarded	No. person months awarded	No. projects started	No. projects completed	No. final reports received	Notes
eCSE01	19	14	132	14	14	14	
eCSE02	17	9	82	9	9	8	1 late final report is being pursued.
eCSE03	16	10	96	10	9	7	1 late final report is being pursued. The final report for the other completed project is not due yet.
eCSE04	16	8	82	8	6	5	1 late final report is being pursued.
eCSE05	14	8	94	8	7	5	The final report for the completed projects are not due yet.

eCSE06	9	5	47	5	2	1	The final report for the completed project is not due yet.
eCSE07	16	5	49	5	0	0	
eCSE08	21	8	88	7	0	0	
eCSE09	19	5	62	0	0	0	
Total	**147**	**72**	**732**	**66**	**47**	**40**	

- A risk analysis is carried out on all successful proposals. For the two most recent calls (eCSE08 and eCSE09), all projects were identified as having either low or very low risk, apart from the following:
  - eCSE08-9 was identified as being of medium risk due to a change of staffing.
    - The new staff member has been approved by the Panel Chair and the project is now awaiting the signing of the contract. We will monitor this to ensure the project gets underway and progresses successfully.
  - eCSE08-10 was identified as being of medium risk due to issues raised by Cambridge University involving the IP and the relationship with the CASTEP group.
    - These issues appear to have been resolved as a contract has recently been signed, but we will monitor this as the project progresses.
  - eCSE09-8 was identified as being of medium risk due to having been awarded 19 person months. This is a higher level of effort awarded than for any other eCSE project, where 15 person months was the previous highest.
    - Of the 19 months awarded for this project, 7 are for a member of the ARCHER CSE team and the work will be monitored through EPCC's standard project monitoring processes. The remaining 12 are for an external member of staff at the PI's institution and will be monitored via regular contact with the PI.
- The following ARCHER webinars were given on completed eCSE projects (the first two were given as a joint session):
  - 19 October 2016 - eCSE04-07 – "Multi-resolution modelling of biological systems in LAMMPS", *Iain Bethune and Oliver Henrich*
  - 19 October 2016 - eCSE05-10 – "Multi-resolution modelling of biological systems in LAMMPS", *Iain Bethune and Oliver Henrich*
  - 9 November 2016 – eCSE05-14 – "Large-Eddy Simulation Code for City Scale Environments", *Z Tong Xie and Vladimir Fuka*
  - 23 November 2016 – eCSE06-6 – "CP2K: Recent performance improvements and new TD-DFT functionality", *Iain Bethune and Matthew Watkins*
  - 30 November 2016 - eCSE03-9 - "Adjoint ocean modelling with MITgcm and OpenAD", *Dan Jones and Gavin Pringle*

eCSE Call 10

- The eCSE10 call opened on 6 December 2016 and will close on 31 January 2017

Future eCSE Calls

- eCSE calls are run to a regular schedule. The future calls are:
  - eCSE11: opens 28 March, 2017 and closes at 4pm on Tuesday 9 May, 2017
  - eCSE12: opens 1 August, 2017 and closes at 4pm on Tuesday 12 September, 2017