ARCHER CSE Service Quarterly Report

Quarter 2 2015

1. Executive Summary

This report covers the period: 1 April 2015 to 30 June 2015 inclusive.

- Centralised CSE Team:
  - Screencasts have been added to the ARCHER YouTube channel and website covering a range of topics. These are designed to allow all users to improve their use of the service and simplify use of advanced features.
  - ARCHER CSE Service staff presented papers at the Exascale Applications and Software Conference (EASC) 2015 and at Cray User Group (CUG) 2015.
  - Two ARCHER White Papers have been published: one on historical usage of UK HPC services that will be of general interest; and a technical paper on use of Cray's RSIP technology that will be of interest to users who want to run commercially licensed software on ARCHER.
  - The CSE Service has begun to share the knowledgebase resulting from answering In-Depth queries through the StackOverflow website. This easily searchable resource will disseminate the experience gained on technical questions throughout the HPC community in the UK and worldwide.

- eCSE:
  - All 14 projects from the 1st eCSE call have started, with 7 now finished. All 9 projects from the 2nd eCSE call have now started, with 2 now finished. From the 3rd call, 8 of the 10 accepted projects have started, and from the 4th call, 5 of the 9 accepted projects have started.
  - The final report template has been updated to request more information on the social, economic and/or academic impact of each project; two completed reports have been received.
  - The 5th eCSE call opened on 31 March 2015 and closed on 12 May 2015; 15 proposals were received, one of which the PI decided to defer. At the Panel meeting held on 23 June 2015, 8 of these projects were accepted.
  - Interim reports have been collected for running eCSE projects. The third eCSE webinar took place in April.
  - One eCSE case study has been produced on "Bone Modelling;" this will be publicised shortly.

- Training:
  - Provided 21 days (267 student-days) of face-to-face training in the quarter, at 8 different locations, with an average feedback score better than "very good".
  - Provided 2 days of virtual tutorials as live interactive webinars; all material was also designed to be used as online training material on the ARCHER web site.
  - Two of the virtual tutorial sessions will be recommended background material for an upcoming face-to-face course.
  - Online training material enhanced with 23 videos of a full 3-day MPI course.
  - Working with ARCHER Outreach project to ensure upcoming "Scientific Computing'' webinars are easily accessible.
  - Course on GPU programming delivered by Sheffield staff using ARCHER material with on-site support from CSE team.
  - 70 eligible users have successfully completed the ARCHER Driving Test; of these, 43 now have ARCHER accounts and have used in excess of 9,000 kAUs.

- ARCHER Outreach Project:
  - Wee ARCHIE: the design of the supercomputer demonstrator, to be constructed from Raspberry PIs, has been completed. Construction will start shortly.
  - The 'Supercomputer App', has been designed and a prototype constructed.
  - The first ARCHER 'Porting and Optimisation Workshop' was run at the beginning of the reporting period, helping attendees with a range of problems from helping users access ARCHER for the first time and use packages to porting, debugging or optimising their own software.

- The second Women in HPC 'Hands on introduction to HPC' workshop was run in Dublin in collaboration with the PRACEDays15 conference, providing female-led training on using HPC and ARCHER.
- Four case studies produced and are available on the web site in an appropriate ARCHER format.

2. Impact Summary

- Outreach Activities:
  - I'm a Scientist, get me out of here!, Online, June 2015: https://www.epcc.ed.ac.uk/blog/2015/06/26/im-scientist-and-im-out-there
  - Edinburgh International Science Festival, National Museum of Scotland, April 2015: http://www.epcc.ed.ac.uk/blog/2015/05/25/day-or-five-museum
  - Sciennes Primary Summer Science Fair, Edinburgh, June 2015: http://www.epcc.ed.ac.uk/blog/2015/06/06/epcc-sciennes-primary-summer-science-fair
  - "Supercomputers = Super Science!", Borders Science Festival, Galashiels, May 2015:
  - http://www.borders-science-festival.org.uk/bsf-archer-may15

- Meetings Attended by Centralised CSE Team:
  - EPSRC RAP, Swindon, 27 May 2015: provided technical and system usage advice to panel.

- Presentations by Centralised CSE team:
  - HPC-SIG, Birmingham, 2 June 2015: presented on ARCHER Champions programme and discussed online training requirements.

- Conference Papers:
  - Adrian Jackson, Toni Collis and Graeme Ackland, GPU Porting with Directives, EASC 2015, Edinburgh, UK, 21-23 April 2015
  - David Henty, Adrian Jackson, Charles Moulinec and Vendel Szeremi, Performance of Parallel IO on Lustre and GPFS, EASC 2015, Edinburgh, UK, 21-23 April 2015
  - Turner, A. R., Parallel Software usage on UK National HPC Facilities, CUG 2015, Chicago, USA, 26-30 April 2015
  - Bareford, M. R., Molecular Modelling and the Cray XC30 Power Management Counters, CUG 2015, Chicago, USA, 26-30 April 2015
  - Pringle, G., Performance and Extension of a Particle Transport Code using Hybrid MPI/OpenMP Programming Models, CUG 2015, Chicago, USA, 26-30 April 2015

- Posters:
  - Iain Bethune, Toni Collis, Mike Jackson, Lennon Ó Náraigh, Prashant Valluri, David Scott, Developing a scalable and flexible code for high resolution DNS of two-phase flows, EASC 2015, Edinburgh, UK, 21-23 April 2015 (won the NVIDIA prize for best poster)
  - Athina Frantzana and Toni Collis, Gender Inequality in HPC and its Effect on the Road to Exascale, EASC 2015, Edinburgh, UK, 21-23 April 2015

3. Forward Look

- Sharing Technical Expertise:
  - We will investigate the possibility of collaborating with other Cray sites in the UK (ECMWF, Met Office) to set up a forum for sharing technical expertise between technical staff.
  - We plan to expand the use of StackOverflow to disseminate technical information.
- Documentation:
  - Implementing Data Management Guide to help users deal with the increasing problems faced by large amount of data (and files) generated from simulations.
  - Additional of a Python chapter to the ARCHER Best Practice Guide to help users understand better how to use Python for both data analysis and modeling on ARCHER.
- Early career researchers as observers at eCSE panel meetings:
  - We would like to invite early career researchers to sit in on future eCSE panel meetings as observers.
  - Seeing how the panel works in practice and what reviewers' value would provide them with invaluable experience that will aid them in writing their own successful proposals.
- Training:
  - Second long-term training impact survey has been issued; this will be analysed and reported in the Q3 report.
  - Planning to attend "8th European Conference on Python in Science" in Cambridge to inform content of upcoming ARCHER "Scientific Python" course.
  - Work with ARCHER Outreach Project to design format and content of Q4 "Scientific Computing" online course to ensure accessibility.
  - Investigate use of pre-configured virtual machines to enable users of online training to undertake practical examples on their laptop without access to HPC resources.
- Outreach
  - In July, Women in HPC will run a workshop and Birds of a Feather session at ISC 2015
  - Women in HPC workshop UK will run in London on 4th September.
  - ARCHER Champions Workshop will run in October 2015 to enable a broad range of attendees.
  - Work commencing on improving accessibility to training courses.
  - Next set of case studies will focus on completed eCSE and RAP projects.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: April 2015, May 2015 and June 2015.

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	Apr-15		May-15		Jun-15		Q2 2015	
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	100%	-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

All metrics were achieved at 100% in this quarter.

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	Apr-15		May-15		Jun-15		Q2 2015	
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	Apr-15	May-15	Jun-15
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 324 queries were resolved by the CSE service in the reporting period.

Metric	Apr-15	May-15	Jun-15	Total	% Total
In-Depth	10	9	23	42	12.1%
Course Registration	151	58	49	258	74.4%
Technical Assessment: Grant	12	5	2	19	5.5%
Technical Assessment: RAP	13	0	0	13	3.7%
Technical Assessment: Instant	1	3	3	7	2.0%
eCSE Application	0	6	2	8	2.3%

All of the feedback left by users on queries was rated "Excellent". 8 query feedback responses were received on In-depth queries in the reporting period. This represents a 19% return rate for feedback forms. This is a large improvement on the return rate from the previous quarter (6%).

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	20	47.6%
User Programs	3	7.1%
Compilers and system software	1	2.4%
Batch System and Queues	1	2.4%
Other	17	10.5%

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 report period.

Q537815: basemap toolbox for matplotlib 1.4.3-python3: A requirement for data analysis using the python 3 software lead to up to date installations of the Anaconda Python framework (https://store.continuum.io/cshop/anaconda/) with all the required components. This benefits all users who need to use Python to analyse data on ARCHER. In addition, this query has lead to a review of the policy for providing Python on ARCHER and this, in turn, has resulted in a more coherent policy and the initiation of work to provide Python-specific documentation on ARCHER to form a new chapter in the ARCHER Best Practice Guide. We also used information gathered in this query to help inform our response to Cray who are currently gathering requirements around Python provision on their systems. As Python continues to grow in popularity among researchers and HPC users all ARCHER users will benefit from rationalisation and documentation on the Python setup on ARCHER.

Q498418: Installing Desmond. The Desmond molecular dynamics software (https://www.deshawresearch.com/resources_desmond.html) is a novel application that has

been designed to simulate biological systems over long time scales. The code has been compiled and tested on ARCHER and made available to all ARCHER users (once they agree to the software Terms and Conditions) through a centrally available module. This installation continues to increase the range of tools available on ARCHER for biomolecular simulations; making the Service more useful for this growing field on the national HPC service.

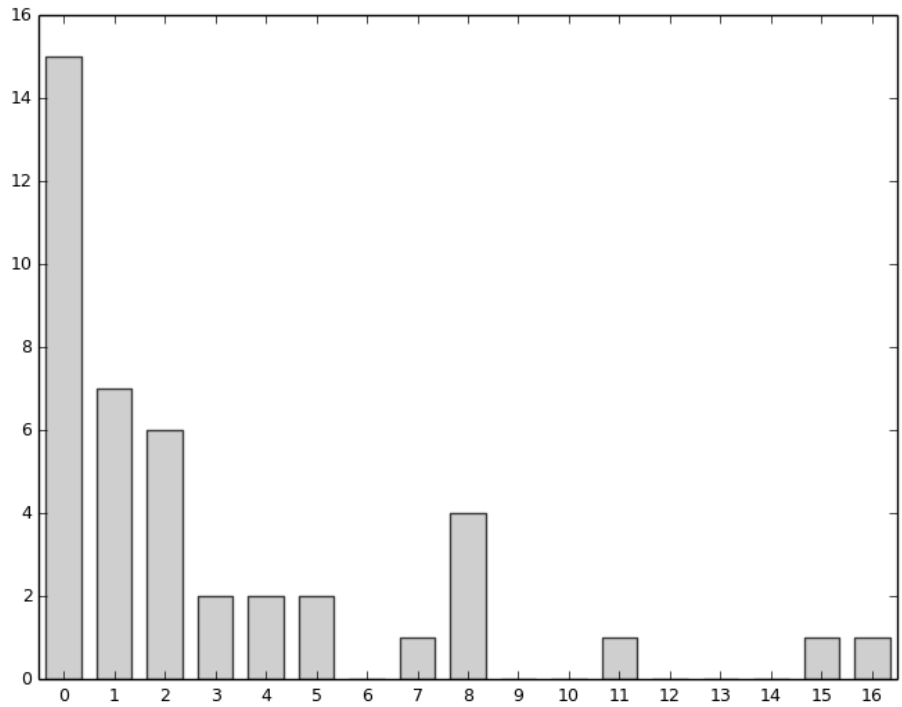
Set up Python environment for NOC analysis: help user and also suggested useful ways to improve Python support on ARCHER going forwards.

Q516413: VASP Problem. An ARCHER user was encountering a problem with the default installation of VASP 5 on ARCHER that lead to segmentation faults after a certain amount of time when running core shift calculations. Investigations by the CSE team revealed that this was due to a memory leak in the code. Various solutions were tried with the resolution being to compile the VASP code with the Intel compiler rather than the GNU compilers. Further tests revealed that the ,latest versions of the Intel compiler on ARCHER produced a version of VASP that had significantly improved performance over the GNU-compiled versions. The central installation was changed to use the executables produced by the Intel compiler passing on these performance benefits to all VASP users on ARCHER. The compilation instructions on the ARCHER website were also updated with the new procedure so that all VASP users on Cray XC systems around the world have the information required to compile an optimal version of VASP. Finally, a note on this was contributed to the community website StackOverflow to disseminate this information as widely as possible.

As VASP accounts for over 15% of all time used on ARCHER the performance improvements are significant benefits to the service.

In-Depth Query Resolution Times

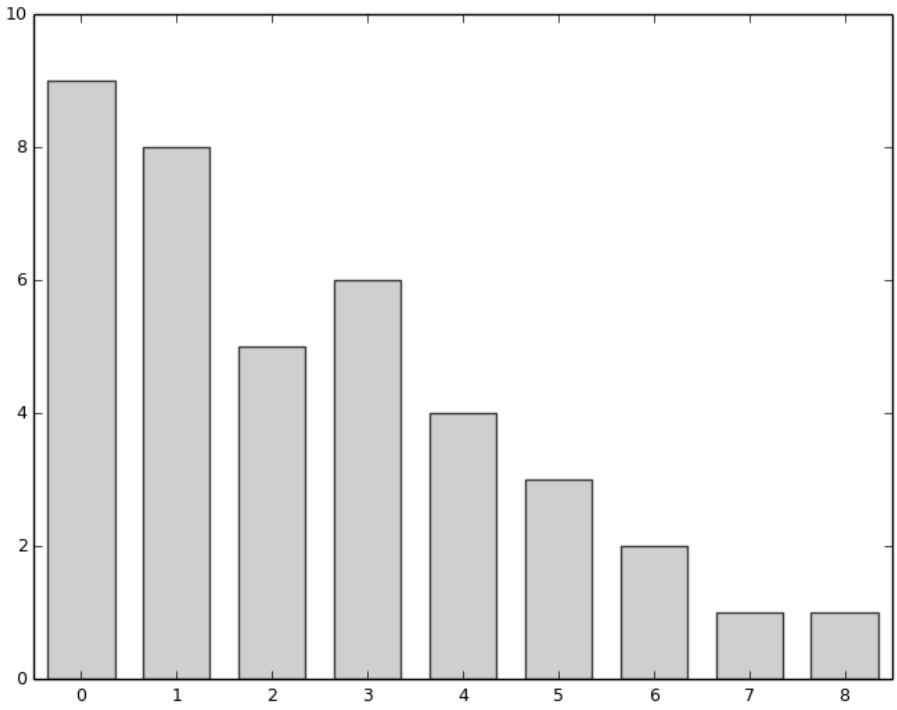
The histogram below shows the time to resolution for In Depth queries in the current reporting period. The median resolution time during this period is 1 week (median resolution time since 1 Jan 2014 is 3 weeks).



Technical Assessment Completion Times

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). There were 37 Technical Assessments requested this quarter compared to 84 in the previous quarter. This decrease is due to the lack of either a RAP or Leadership call in this quarter. Number of Technical Assessments completed by quarter so far:

- Q1 2014: 23
- Q2 2014: 51
- Q3 2014: 61
- Q4 2014: 38
- Q1 2015: 84
- Q2 2015: 37



6. Training

The CSE Service has provided a total of 21 days (374 student-days) of face-to-face training across eight different locations in the reporting period, plus 2 days of interactive web-based training.

Month	Dates	Course	Location	Days	Attendees
Apr 2015	8	Single Node Performance Optimisation - Part 1	Online	0.5	
	14-16	Message-Passing Programming with MPI	Southampton	3	33
	15	Single Node Performance Optimisation - Part 2	Online	0.5	
	16-17	Software Carpentry Workshop	London	2	24
	28-29	Multicore Programming	Edinburgh	2	17
	30-01	Programming the Xeon Phi	Edinburgh	2	15
May 2015	5	GPU Programming	Sheffield	1	20
	7-8	Fortran 95	Oxford	2	13
	20-21	Single-sided PGAS Communications Libraries	Bristol	2	5
Jun 2015	3	Introduction to Version Control - Part 1	Online	0.5	
	17	Introduction to Version Control - Part 1	Online	0.5	
	22-23	Programming the Xeon Phi	Southampton	2	13
	25-26	Performance Analysis Workshop	Durham	2	18
	29-01	Introduction to Molecular Dynamics on ARCHER	Glasgow	3	15

The "Message-Passing Programming" course in Southampton included students from their CDT in Next-Generation Computational Modelling. These students will receive accreditation for this course from Southampton University, based on successful completion of exercises set by EPCC. Three of this quarter's courses ("Multicore Programming" and "Programming the Xeon Phi" in EPCC, "Performance Analysis Workshop" in Durham) were jointly organised between the ARCHER and DiRAC services, providing added benefit to both user communities. Machine access to both services was offered to all attendees, and the cost of hosting and presenting the courses has also been shared. The "GPU programming" course in Sheffield was delivered by local staff using ARCHER material, supported by a CSE team member who assisted with practical sessions.

On the feedback forms, 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 4.2. i.e. better than "Very Good". Users provided 64 feedback forms on the CSE courses, a response rate of 37%.

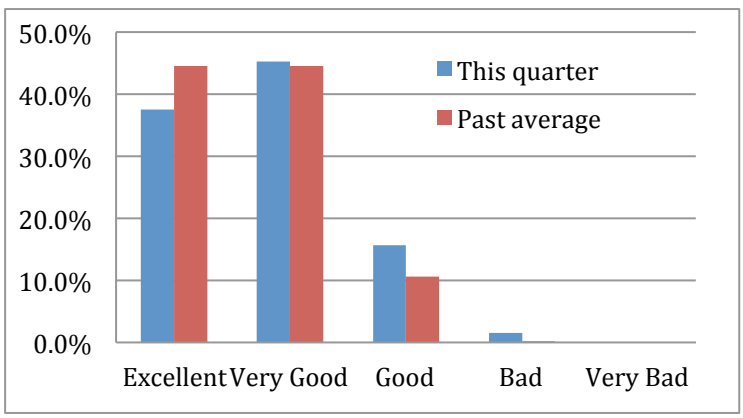


Figure 1: Breakdown of feedback responses from training course surveys for Q2 2015.

The response rate is lower than normal (e.g. last quarter it was 50%). However, three courses were run in the final week of June and we are still receiving feedback from them.

A total of 16 days of face-to-face training are currently planned for the next quarter, plus 1.5 days of online courses. Details are provided in the table below.

Month	Dates	Course	Location	Days
Jul 2015	2-3	Advanced OpenMP	Manchester	2
	13-14	Hands-on Introduction to HPC	Edinburgh	2
	8	Virtual tutorial: Building codes with make	Online	0.5
	15-17	Message-Passing Programming with MPI	Edinburgh	3
Aug 2015	TBC	Data Carpentry	Leeds	2
	12	Virtual tutorial: tips and tricks for using bash	Online	0.5
	TBC	Performance Programming	Bristol	2
Sep 2015	1-3	Message-Passing Programming with MPI	Southampton	3
	9	Virtual tutorial: title TBC	Online	0.5
	TBC	Shared-Memory Programming with OpenMP	London	2

Online Training

We have extended the provision of online training in a number of ways:

- The "Single-node Performance Optimisation" virtual tutorial is also available online and is designed to be studied by students in advance of the upcoming "Performance Programming" course in Bristol. This has enabled us to streamline the face-to-face course as we can now ensure that all attendees have more comparable baseline knowledge when they arrive.
- The "Introduction to Version Control" virtual tutorial was delivered in two parts to give students time to practice the basic material from the first tutorial before attending the second. All this material is now online, with an associated online practical example for students to attempt between the two presentations.
- An entire 3-day run of the "Message-Passing Programming" course from the 2014 ARCHER Summer School is now available as a youtube playlist of 23 videos, linked in from the ARCHER web pages with all associated slides, lecture notes and example codes.
- We have progressed plans for the introductory online course on "Scientific Computing" to be delivered as four half-day webinars over four weeks in October/November. This will be delivered live to CDT students on the "Pervasive Parallelism" CDT in Edinburgh, streamed live for online attendees, and recorded for the ARCHER website. We are working closely with the ARCHER Outreach project to ensure that this course is easily accessible to remote attendees. We plan to support this course with at least one virtual tutorial to allow remote attendees to actively engage with ARCHER staff.

The ARCHER Driving Test is proving to be a popular mechanism for new users to access the system. The statistics so far are (those from last quarterly report in brackets):

- 70 (45) eligible users have successfully completed the ARCHER Driving Test;
- of these, 43 (28) now have ARCHER accounts;
- they have used in excess of 9,000 (4000) kAUs.

7. Outreach Project

This reporting period covers the kick-off of the ARCHER Outreach project and its activities, as well as the on-going Women in HPC programme of events.

During this period work has begun on the following projects:

- Wee ARCHIE, the mini-supercomputer, has been through an initial design phase. The cluster will consist of 16 worker Raspberry Pis plus two management Pis. Each Pi will be fronted by an LED 8x8 matrix to initially show the load on that Pi at any given time. The matrices will be pure green LEDs driven by the i2c protocol via the GPIO pins on the Raspberry Pis. This has been tested to work using a generation one Raspberry Pi and will be adapted to the Gen 2 models shortly.
- We are working on a beta version of a 'Supercomputer App' that will be usable by the general public, both at science festivals and for use at home, with the aim of demonstrating some of the compenents of a supercomputer and the trade-offs considered when purchasing them, in order to raise public interest in supercomputing. The app will enable the public to 'build' their own supercomputer and see how much science they could run on it subject to a budget. An initial prototype has been completed and a beta version is in progress.
- Four case studies have been completed and are now available on the ARCHER website:
  - Modelling blood flow around the vessels of the brain',
  - 'Extreme weather forecasting with extreme computing'
  - 'Aircraft Research Association Ltd'
  - 'Albatern: Numerical simulations of extremely large interconnected wave arrays'

ARCHER outreach has also completed two events, spanning 3 days during this period:

- Porting and Optimisation workshop ("hackathon") – Edinburgh, UK;
- Women in HPC Hands-on Introduction to HPC – Dublin, Ireland.

The 'hackathon' was referred to as a 'Porting and Optimisation workshop' as initial investigation suggested that referring to events as 'hackathon' can have a detrimental impact on the diversity of attendees. The workshop was set up as a full-day event providing tailored, one-to-one assistance to attendees. The attendees ranged from completely new users who were able to use ARCHER for the first time and who received advice on gaining access to ARCHER to competent users who asked for advise on optimising software. The ARCHER CSE team provided one member of technical staff for each pair of attendees.

Feedback for the workshop was received from 9 of the 18 participants. On the feedback forms, attendees rated the course on a scale of 1-5 ("Very bad", "Bad", "Good", "Very good" and "Excellent"): all attendees rated the workshop as 'Excellent'. The feedback also suggested that the attendees appreciate the high staff to attendee ratio, and the 'freeform' surgery nature of the event.

Women in HPC

During this reporting period the Women in HPC initiative has significantly improved its social media presence, reaching 445 twitter follows, from a previous peak of 315 on 31 March 2015. The network now has 172 newsletter subscribers, including 26 new subscribers during this reporting period.

The 'Women in HPC workshop: A hands-on introduction to HPC' was held in May in Dublin, in collaboration with the PRACEDays 2015 conference. The purpose of the workshop was to provide a female-led workshop with a predominantly female audience.

The workshop had 18 attendees, including 2 men and 16 women. Feedback from the workshop was received from 12 of the attendees. On the feedback forms, attendees rated the course on a

scale of 1-5 ("Very bad", "Bad", "Good", "Very good" and "Excellent"): all attendees rated the workshop as either as 'Excellent' or 'Very good' with an average of 4.3 (i.e. above 'Very Good'). The feedback also highlighted that the attendees appreciated a female-led course. When asked 'what did you like the most about the course', some of the responses included:

- "1st workshop conducted by a woman HPC"
- "You could follow the practicals at your own pace and not feel rubbish if you were a bit slow"
- "The environment, which was very relaxed and casual and friendly. I felt the provision of a course run by women reduced the assumptions made about prior knowledge or computing experience and made the session more accessible to people of all levels."
- "Knowing that this course would be mostly women did make attending far less intimidating."

Case Studies:

Throughout the period the outreach project has created four new case studies, developing a standard style and format; this will be continued throughout the project. These case studies are available on the ARCHER web site. The project also worked with the eCSE team to produce a first eCSE case study, for the bone modeling work (VOX-FE code) carried out by the University of Hull and EPCC. Publicity for this case study is currently being discussed. The next set of case studies will look to completed eCSE and RAP projects.

Upcoming events:

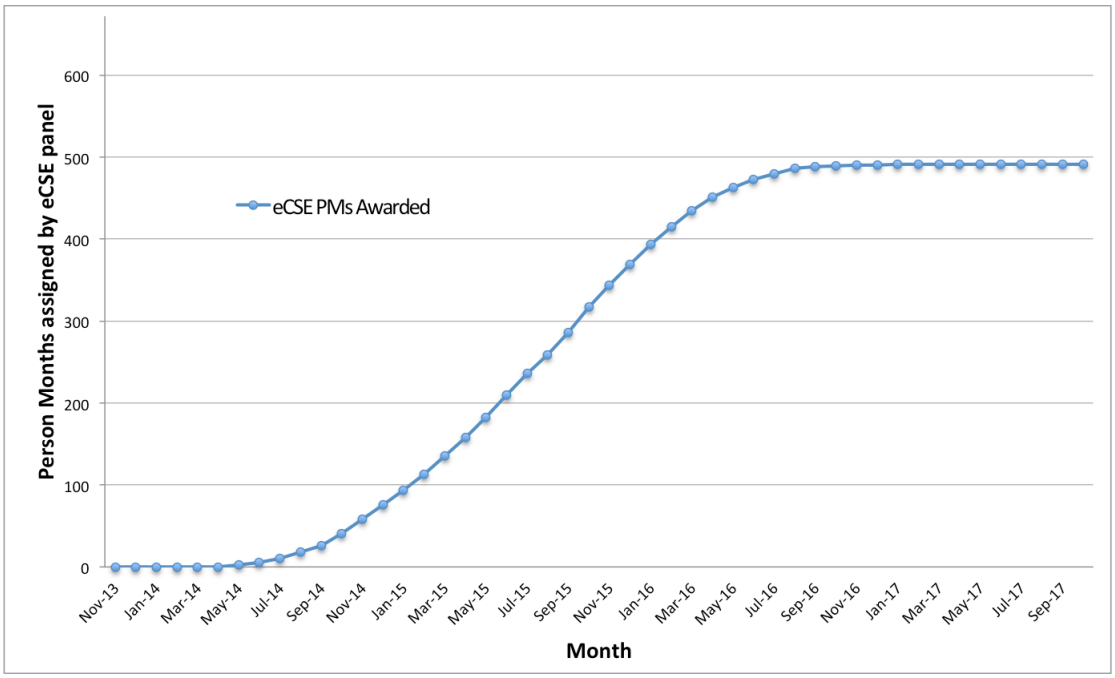
Women in HPC will have the following events in 2015 Q3:

- Women in HPC workshop at ISC 2015, 16 July 2015;
- Women in HPC BoF: 'How can the HPC industry benefit from the diversity dividend' at ISC 2015, 14 July 2015;
- Women in HPC in the UK, London, 4 September 2015.

There will also be an "ARCHER Champions" workshop in early October.

8. Embedded CSE (eCSE)

Overview of eCSE Effort



- The eCSE person months awarded up to and including the 4th eCSE call are shown above
- At least 672 person months will be awarded by the end of the project (14 FTEs for 4 years)
- 492 person months have been awarded so far over 50 awarded eCSE projects
- We expect future eCSE Panels to allocate about 50 PMs each. The last full eCSE Panel meeting is planned to be about 1 year before the end of ARCHER.

eCSE Call 1

- All 14 projects have started and contracts have been agreed and signed where needed
- A risk analysis identified all projects as being of either low or very low risk apart from eCSE01-019 which was considered to be of medium risk due to difficulties in agreeing staffing for the project.
    - This project has now started and progress is being monitored via the eCSE contact within the centralised CSE team

eCSE Call 2

- All 9 projects have started and contracts have been agreed and signed where needed
- A risk analysis identified all projects as being of either low or very low risk apart from the following:
    - eCSE02-2 which was considered to be of medium risk due to its reliance on outdated versions of OpenFOAM. The technical staff member for this project is in the process of moving the work to more recent versions of OpenFOAM.
        - This is being monitored via the eCSE contact within the centralised CSE team with a number of meetings having taken place. The project appears to be progressing well.
    - eCSE02-11 which was considered of medium risk due to the original named member of technical staff leaving the project and a new member of staff being recruited.

        - This project has been paused as the member of staff left after 6 weeks. The PI is in the process of identifying a replacement member of staff

eCSE Call 3

- 8 of the 10 projects have started
- 6 projects require contracts. 1 has been signed; 5 are presently in the process of being negotiated
- A risk analysis identified all projects as being of either low or very low risk apart from the following:
    - eCSE03-8 which was identified as being of medium risk due to the challenging nature of completing the work within the given timescale
        - This project appears to be progressing well
    - eCSE03-9 which was identified as being of medium risk due to the technically challenging nature of the work
        - This project appears to be progressing well

eCSE Call 4

- 5 of the 9 projects have started
- 6 projects require contracts. 3 have been signed; 1 is presently in the process of being finalised
- A risk analysis identified all projects as being of either low or very low risk apart from the following:
    - eCSE04-1 which was identified as being of medium risk due to the fact that the number of person months was cut from 10 in the original proposal down to 6 funded, and the acceptance of the project is dependent on a new workplan being agreed.
        - This project was accepted conditionally and is still under discussion
    - eCSE04-4 which was identified as being of medium risk as the person named to do the technical work has been offered a position elsewhere.
        - The member of staff originally named on the contract will be able to complete 3 of the 12 months of work. We are presently discussing with the PI possibilities for staffing the remainder of the work
    - eCSE04-10 which was identified as being of medium risk as the PI has indicated that the person named to do the technical work may not be available.
        - This is presently under discussion with the PI
    - eCSE04-16 which was identified as being of medium risk as the PI has indicated that the person named to do the technical work may not be available..
        - This is presently under discussion with the PI

eCSE Call 5

- The 5th eCSE call opened on 31st March and closed on 12th May
- 15 proposals were received requesting a total of 161 person months. One project has since deferred due to the member of staff leaving since the proposal was submitted
- At the Panel meeting on 23 June 2015 8 projects were accepted funding a total of 93 person months
- A number of improvements were made for this call. For example:
    - The proposal form now contains sections for stating whether a proposal is a follow-on proposal or a re-submission
    - The proposal form now requires the identification of the involved ARCHER consortia
    - Guidance on what a New Community is has been improved

Future eCSE Calls

eCSE calls are run to a regular schedule. The future calls are:

- eCSE06: opens Tuesday 04/08/15 and closes at 4pm on 15/09/15
- eCSE07: opens Tuesday 24/11/15 and closes at 4pm on 19/01/16
- eCSE08: opens Tuesday 29/03/16 and closes at 4pm on 10/05/16
- eCSE09: opens Tuesday 02/08/16 and closes at 4pm on 13/09/16

eCSE Call 1: Project List

eCSE ID	PI	Title	Tech staff institution (PMs/Inst)	PMs	Status
eCSE01-001	Michail Stamatakis <m.stamatakis@ucl.ac.uk> (UCL)	*Zacros Software Package Development: Pushing the Frontiers of Kinetic Monte Carlo Simulation in Catalysis*	Dr Owain Kenway (3/UCL); Dr Ian Kirker (3/UCL); Dr Jens Nielsen (3/UCL); Dr Mayeul d'Avezac (3/UCL)	12	started 01/09/2014 finishes 31/08/2015
eCSE01-002	Dr Alan Gray < a.gray@ed.ac.uk> (EPCC)	*Introducing Thread and Instruction Level Parallelism into Ludwig*	Alan Gray (12/EPCC)	12	started 01/09/2014 finishes 31/08/2016
eCSE01-003	Dr Benedict Rogers <benedict.rogers@manchester.ac.uk> (Manchester)	*Developing highly scalable 3-D incompressible SPH*	Dr Xiaohu Guo (12/STFC)	12	started 01/09/2014 finishes 31/08/2015
eCSE01-004	Chris-Kriton Skylaris <c.skylaris@soton.ac.uk> (Southampton)	*A pinch of salt in ONETEP's solvent model*	Lucian Anton (2/STFC); Jacek Dziedzic (1/Southampton)	3	finished 31/10/2014
eCSE01-005	Mark van Schilfgaarde <mark.van_schilfgaarde@kcl.ac.uk> (KCL)	*QuasiParticle Self-Consistent GW calculations of many-atom systems*	Martin Lueders (3/STFC); Leon Petit (3/STFC)	6	started 01/08/2014 finishes 31/07/2015
eCSE01-008	Dr. Prashant Valluri <Prashant.Valluri@ed.ac.uk> (Edinburgh (non EPCC))	*TPLS: Optimised Parallel I/O and Visualisation*	Toni Collis (8/EPCC)	8	finished [1] 31/01/2015
eCSE01-009	Dr Gerard Gorman<g.gorman@imperial.ac.uk> (Imperial)	*Scalable and interoperable I/O for Fluidity*	Dr Michael Lange (6/Imperial)	6	finished 31/12/2014

[1] Final report received

eCSE01-010	Dr Miguel O. Bernabeu<miguel.bernabeu@ucl.ac.uk> (UCL)	*Adding a resolved deformable particle model to a highly-parallel blood flow solver for sparse vascular networks*	Dr Owain Kenway (3/UCL); Dr Ian Kirker (3/UCL); Dr Jens Nielsen (3/UCL); Dr Mayeul d'Avezac (3/UCL)	12	started 01/09/2014 finishes 31/08/2015
eCSE01-013	Jimena Gorfinkiel <Jimena.Gorfinkiel@open.ac.uk> (Open)	*Efficient computation of two-electron integrals in a mixed Gaussian/B-spline basis.*	Zdenek Masin (12/Open)	12	finished 31/05/2015
eCSE01-015	Professor Michael J Fagan <m.j.fagan@hull.ac.uk> (Hull)	*Large scale voxel based modelling*	Dr Neelofer Bangawala (7/EPCC); Dr Richard Holbrey (8/Hull)	15	finished [1] 31/03/2015
eCSE01-016	Dr Massimo Bollasina<massimo.bollasina@ed.ac.uk> (Edinburgh (non EPCC))	*Porting and enabling use of the Community Earth System Model on ARCHER*	Gavin Pringle (4/EPCC)	4	finished 30/11/2014
eCSE01-017	Dr Matt Probert <matt.probert@york.ac.uk> (York)	*Hybrid OpenMP and MPI within the CASTEP code*	Edward Higgins (12/York)	12	started 01/07/2014 finishes 30/06/2015
eCSE01-018	Scott M. Woodley <Scott.Woodley@ucl.ac.uk> (UCL)	*Tuning FHI-Aims for complex simulations on CRAY HPC platforms*	Matthew Farrow (12/UCL)	12	finished 31/05/2015
eCSE01-019	lian Todorov <Ilian.todorov@stfc.ac.uk> (STFC)	*DL_POLY_4: Multiple Time Stepping Development Support*	Ian Bush (6/Oxford)	6	started 01/01/2015 finishes 31/03/2016

eCSE Call 2: Project List

eCSE ID	PI (Institution)	Title	Technical Staff (PMs/Institution)	PMs	Status
eCSE02-2	Prof Jason M Reese <jason.reese@ed.ac.uk> (Edinburgh (non EPCC))	*Multi-Scale Engineering Flow Simulation: Hybrid MPI/OpenMP Optimization on ARCHER*	Saif Mulla (12/Edinburgh (non EPCC))	12	started 01/09/2014 finishes 31/08/2015
eCSE02-3	Dr. Patrick E. Farrell<patrick.farrell@maths.ox.ac.uk> (Oxford)	*Scalable automated parallel PDE-constrained optimisation for dolfin-adjoint*	Dominic Sloan-Murphy (8/EPCC)	8	started 01/09/2014 finishes 30/06/2015
eCSE02-6	Prof Hugo van der Hart <h.vanderhart@qub.ac.uk> (QUB)	*Performance enhancement of RMT codes in preparation for the treatment of circular polarization*	Jonathan Parker (9/QUB)	9	started 01/10/2014 finishes 30/06/2015
eCSE02-8	Dr David Dickinson<d.dickinson@york.ac.uk> (York)	*Optimising Field Solvers in GS2: Improved load balancing and non-blocking communications for maximal efficiency at high #core*	Adrian Jackson (7/EPCC)	7	started 01/09/2014 finishes 30/06/2015
eCSE02-9	Matt Probert <matt.probert@york.ac.uk> (York)	*Optimising van der Waals simulations with the CASTEP code*	Matthew Hodgson (7/York)	7	finished 31/03/2015
eCSE02-11	Dr Nicolae Panoiu <n.panoiu@ucl.ac.uk> (UCL)	*Fast and Massively Distributed Electromagnetic Solver for Advanced HPC Studies of 3D Photonic Nanostructures*	Marcello Artioli (12/UCL)	12	started 01/02/2015 finishes 31/01/2016
eCSE02-13	Prof Spencer Sherwin<s.sherwin@imperial.ac.uk > (Imperial)	*Communication and I/O masking for increasing the performance of Nektar++*	Simon Clifford (6/Freelance); Rupert Nash (6/EPCC)	12	started 01/10/2014 finishes 30/09/2015

eCSE02-15	Dr Nicholas D M HINE <ndmh3@cam.ac.uk> (Cambridge)	*Calculating Excited States of Extended Systems in LR-TDDFT*	Tim Zuehlsdorff (6/Cambridge)	6	finished 31/03/2015
eCSE02-17	Dr James Harle <jdha@noc.ac.uk> (NOC)	*NEMO Regional Configuration Toolbox*	Srikanth Nagella (6/STFC); Shirley Crompton (3/STFC)	9	started 01/10/2014 finishes 30/09/2015

eCSE Call 3: Project List

eCSE ID	PI (Institution)	Title	Technical Staff (PMs/Institution)	PMs	Status
eCSE03-1	Prof. Tony Arber <t.d.arber@warwick.ac.uk> (Warwick)	*Optimisation of the EPOCH laser-plasma simulation code*	Michael Bareford (12/EPCC)	12	started 01/01/2015 finishes 31/12/2015
eCSE03-2	Dr. Michele Sergio Campobasso <m.s.campobasso@lancaster.ac.uk> (Lancaster)	*Reducing the run-time and improving the ease-of-use and portability of the COSA 3D harmonic balance Navier-Stokes solver for open rotor unsteady aerodynamics*	Adrian Jackson (7/EPCC)	7	started 01/04/2015 finishes 31/03/2016
eCSE03-3	Dr David J Huggins <djh210@cam.ac.uk> (Cambridge)	*Algorithmic Enhancements to the Solvaware Package for the Analysis of Hydration*	Arno Proeme (6/EPCC)	6	started 12/01/2015 finishes 30/06/2015
eCSE03-7	Dr Matthew Piggott <m.d.piggott@imperial.ac.uk> (Imperial)	*Delivering a step-change in performance and functionality to the Fluidity shallow water solver through code generation*	Christian Jacobs (12/Imperial)	12	started 01/02/2015 finishes 31/01/2016
eCSE03-8	James R. Maddison <j.r.maddison@ed.ac.uk> (Edinburgh (non EPCC))	*Parallel supermeshing for multimesh modelling*	Iakovos Panourgias (8/EPCC)	8	started 01/01/2015 finishes 31/08/2015
eCSE03-9	Dr Dan Jones <dannes@bas.ac.uk> (BAS)	*Providing the ARCHER community with adjoint modelling tools for high-performance oceanographic and cryospheric computation*	Sudipta Goswami (5/BAS); Gavin Pringle (4/EPCC)	9	started 11/02/2015 finishes 31/10/2015
eCSE03-10	Dr Garth Wells <gnw20@cam.ac.uk> (Cambridge)	*High performance multi-physics simulations with FEniCS/DOLFIN*	Chris Richardson (6/Cambridge)	6	started 01/03/2015 finishes 29/02/2016

eCSE03-11	Dr Matthew B Watkins <matthew.watkins@ucl.ac.uk> (UCL)	*local excitement in CP2K*	Matthew Watkins (12/UCL)	12	starting date TBD
eCSE03-12	Xuerui Mao <xuerui.mao@durham.ac.uk> (Durham)	*Full parallelism of calculations of optimal flow control*	Bofu Wang (12/Durham)	12	starting date TBD
eCSE03-13	Dr Rupert Nash <rupert.nash@ed.ac.uk> (EPCC)	*Grids in grids: hierarchical grid generation and decomposition for a massively parallel blood flow simulator*	Rupert Nash (10/EPCC); Derek Groen (2/UCL)	12	started 01/01/2015 finishes 31/12/2016

eCSE Call 4: Project List

eCSE ID	PI (Institution)	Title	Technical Staff (PMs/Institution)	PMs	Status
eCSE04-1	Mathew Williams <m.williams@ed.ac.uk> (Edinburgh (non EPCC))	*Enabling R users to exploit trivial parallelism on ARCHER*	CSE staff (TBD) (4/EPCC); Thomas L Smallman (2/Edinburgh (non EPCC))	6	Conditional funded. Still under negotiation and waiting for the confirmation. Proposed starting 01/09/2015 finishes 31/12/2015
eCSE04-3	Dr Daniel Dundas <d.dundas@qub.ac.uk> (QUB)	*A photoelectron spectrum library for laser-matter interactions*	Alejandro de la Calle (12/QUB)	12	started 01/04/2015 finishes 31/03/2016
eCSE04-4	Graeme Ackland <gjackland@ed.ac.uk> (Edinburgh (non EPCC))	*Implementing lattice-switch Monte Carlo in DL_MONTE to unlock efficient free energy calculations*	Tom Underwood (12/Edinburgh (non EPCC))	12	started 14/04/2015 finishes 31/03/2016
eCSE04-7	Jonathan Essex <jwe1@soton.ac.uk> (Southampton)	*Implementation of Dual Resolution Simulation Methodology in LAMMPS*	Iain Bethune (6/EPCC)	6	starting 01/08/2015 finishes 31/07/2016
eCSE04-10	Jonathan Yates<(jonathan.yates@materials.ox.ac.uk> (Oxford)	*Large scale CASTEP calculations to interpret solid-state NMR and Vibrational Spectroscopy experiments*	Bi-Ching Shih (12/Oxford)	12	starting date TBD

eCSE04-11	Prof. Michael J Fagan <M.J.Fagan@hull.ac.uk> (Hull)	*VOX-FE - new functionality for new communities*	Dr. Neelofer Banglawala (3/EPCC); Dr. Richard Holbrey (6/Hull)	9	started 01/04/2015 finishes 30/09/2015
eCSE04-13	Dr Charles Moulinec <charles.moulinec@stfc.ac.uk> (STFC)	*Implementation of a highly scalable aeroacoustic module based on the Ffowcs Williams and Hawkings analogy within the open-source CFD software Code_Saturne*	Dr Stefano Rolfo (12/STFC)	12	starting 01/07/2015 finishes 30/06/2016
eCSE04-14	Dr Justin R Finn <J.Finn@liverpool.ac.uk> (Liverpool)	*CFD2LCS: A general purpose library for integrated computation of Lagrangian coherent structures during massively parallel hydrodynamic simulations.*	Dr Justin Finn (10/Liverpool)	10	started 01/04/2015 finishes 31/01/2016
eCSE04-16	Prof Nicholas M Harrison <nicholas.harrison@imperial.ac.uk> (Imperial)	*Removing pseudo-linear dependence in Gaussian basis set calculations on crystalline systems with the CRYSTAL code*	Mr Ross Webster (9/Imperial)	9	starting date TBD

eCSE Call 5: Project List

eCSE ID	PI (Institution)	Title	Technical Staff (PMs/Institution)	PMs	Status
eCSE05-4	Prof George N Barakos <g.barakos@liverpool.ac.uk> (Liverpool)	*Discrete velocity methods for the Helicopter Multi-Block CFD solver*	Mark Woodgate (12/Liverpool); ARCHER CSE(2/EPCC)	14	01/08/2015
eCSE05-5	Dr Anton Shterenlikht <mexas@bris.ac.uk> (The University of Bristol)	*Open source exascale multi-scale framework for the UK solid mechanics community*	Luis Cebamanos(6/EPCC); TBD (6/Manchester)	12	01/09/2015
eCSE05-6	Lucia Sivilotti <l.sivilotti@ucl.ac.uk> (UCL)	*Parallelization and porting of single-channel analysis tools to the high-performance computing platform*	Dr Remigijus Lape(3/UCL); TBD (9/UCL)	12	01/09/2015
eCSE05-7	Dr. Angus Creech <a.creech@ed.ac.uk> (University of Edinburgh)	*Optimisation of Large Eddy Simulation (LES) turbulence modelling within Fluidity*	Dr. Angus Creech (12/Edinburgh)	12	17/08/2015
eCSE05-10	Dr Oliver O Henrich <ohenrich@epcc.ed.ac.uk> (EPCC)	*Adding Multiscale Models of DNA to LAMMPS*	Dr Oliver Henrich (12/EPCC)	12	05/10/2015
eCSE05-12	Dr Paul Connolly <paul.connolly@manchester.ac.uk (Manchester)	Enabling large-scale microphysics and optimising solver performance in MONC	Nick Brown(8/EPCC)	8	01/09/2015
eCSE05-13	Dr Jun Xia <jun.xia@brunel.ac.uk> (Brunel University London)	Optimisation of LESsCOAL for large-scale high-fidelity simulation of coal pyrolysis and combustion	Kaidi Wan(11/Brunel University London)	11	14/09/2015
eCSE05-14	Dr Zheng-Tong Xie <z.xie@soton.ac.uk> (University of Southampton)	Large-Eddy Simulation Code for City Scale Environments	Dr Vladimir Fuka (10/Southampton); ARCHER CSE(2/EPCC)	12	12/08/2015