ARCHER CSE Service Quarterly Report

Quarter 3 2015

1. Executive Summary

This report covers the period: 1 July 2015 to 30 September 2015 inclusive.

- Centralised CSE Team:
    - Initiated contact with Met Office and ECMWF about forming a UK forum for sharing technical expertise on applications on Cray systems. Both organisations are keen to be involved with this.
    - We have continued to add topics to the StackOverflow website to disseminate knowledge and experience gained in the ARCHER CSE Team to as wide a community as possible.
    - A major re-working of the Python environment on ARCHER has been undertaken to improve the user experience with this tool for both modeling and data analysis. The growth of Python is one of the major features of both HPC and data analytics at the moment, and proper support for these tools is now a key part of the ARCHER service.
    - We have started a set of coordinated activities to raise awareness of data management issues amongst ARCHER users and to provide practical advice on dealing with large, complex datasets. These include:
        - Data Management Best Practice Guide
        - Webinars on topics around data management
        - Embedding data management advice into documentation and training
        - Addition of data management plan section to ARCHER TA form
- eCSE:
    - From the 1st and 2nd eCSE calls, 20 of the 23 projects have now completed with 10 final reports received. From the 3rd and 4th eCSE calls, 16 out of 18 projects have now started with 1 project from the 3rd call having completed. From the 5th call, 5 of the 8 projects have started.
    - The 10 final reports received are being reviewed and summaries are being added to the eCSE pages of the ARCHER website.
    - The 6th eCSE call opened on 04/08/15 and closed at 4pm on 15/09/15, receiving 9 proposals that are presently under review.
- Training:
    - Provided 12 days (253 student-days) of face-to-face training in the quarter, at 3 different locations, with an average feedback score better than "very good".
    - Ran 4 virtual tutorials as live interactive webinars with an average of 19 attendees.
    - Draft training plan for 2016 has been sent to the ARCHER Training Panel
    - Second summary report for follow-up survey on longer-term impact of training sent to Training Panel for comment.
    - New "Data Carpentry" course on 29-30 October is already full with 45 registrations.
    - 25 new users gained access in Q3 via the ARCHER driving test; there were 25 such users active this quarter, submitting 2,500 jobs and using 17,000 kAUs.
- ARCHER Outreach Project:
    - Wee ARCHIE: build of the mini-supercomputer demonstrator constructed from 18 Raspberry Pi's has been completed.
    - The 'Supercomputing App' has been completed and tested.
    - A new website promoting diversity in HPC is currently being designed.
    - Faces of HPC project: interviews and biographies of HPC users showcasing the diversity of the community have begun, with 8 completed interviews and 3 historical biographies completed.
    - Women in HPC ran two further workshops in this reporting period: the first as a workshop at ISC15 (Frankfurt, July 2015); the second was a careers workshop for early career women in UK held at the BCS (London, September 2015).
    - ARCHER Champions: a preliminary teleconference was well received. Planning has now commenced for the first face-to-face event for Q1 2016.
    - Five case studies have now been completed and are available online.

2. Impact Summary

- Meetings Attended by Centralised CSE Team:
    - Joint DiRAC Benchmarking/ARCHER CSE Meeting to discuss IO benchmarks and agree joint work going forwards, Sep 2015
    - PRACE Operations Face2Face Meeting, Bologna, Sep 2015

- Presentations by Centralised CSE team:
    - ARCHER Update, UKCTRF Annual Meeting, Imperial College, 22-23 Sep 2015
    - HPC Architectures, EPSRC HPC Autumn Academy, Cambridge, 21 Sep 2015
    - ARCHER and CSE Team Update: EPSRC HEC Chairs Meeting, via Skype, Sep 2015

- Conference Papers:
    - Invited Talk: Developing a scalable and flexible code for high-resolution DNS of two-phase flows", I. Bethune, 2nd ThermaPOWER Mini-symposium, 14th UK Heat Transfer Conference 2015, Sep 2015
    - Parco paper: "Developing a scalable and flexible high-resolution DNS code for two-phase flows", I. Bethune, T. Collis, L. O Naraigh, D. Scott, P. Valluri, International Conference on Parallel Computing (ParCo), Edinburgh, 2015

- Posters:
    - "Developing a scalable and flexible code for high-resolution DNS of two-phase flows", I. Bethune, T. Collis, M. Jackson, L. O Naraigh, P. Valluri, 14th UK Heat Transfer Conference 2015, Sep 2015

3. Forward Look

- UK-RDF:
  - o The ARCHER CSE team will become more involved in providing technical support for the UK-RDF and completing technical assessments for RDF access.
  - o The team will focus on helping people to use the Data Analytic Cluster (DAC) and Data Transfer Nodes (DTNs) to improve research productivity.
  - o Shifting a number of analysis parts of some workflows from ARCHER to the UK-RDF DAC should allow for a wider variety of tools and techniques to be available to ARCHER users to support their research

- Understanding user workflows and current bottlenecks:
  - o To inform development of the ARCHER and UK-RDF services, we would like to have an up-to-date view of the research workflows in use and where the bottlenecks lie. The end-to-end research workflow has become more important as the size and complexity of HPC modelling and simulation has increased.
  - o We are planning a user consultation exercise aimed particularly at the large research Consortia on ARCHER. The first step will be contact with major users via the Consortium Contacts to get a description of their workflows and where they encounter bottlenecks that hinder their research.
  - o Any immediate improvements that can be made to workflows (e.g. automation, optimisation) or the services (batch system configuration, tool availability) to eliminate bottlenecks will be implemented.
  - o We will write a white paper based on this work demonstrating how bottlenecks in HPC workflows can be analysed and eliminated, and noting challenges for the future that can help inform future HPC service procurements.

- ARCHER Technical Assessment Form Update:
  - o Add section on Data Management Plan to ensure applicants have considered the issues around data generated by calculations on ARCHER.
  - o Clarification of job size table to militate potential confusion over pure-MPI vs. hybrid MPI/OpenMP jobs.
  - o Allow users to request ARCHER resources for full term of grant (broken down into 6 month periods) rather than just first two years.

- eCSE:
  - o Allow observers at eCSE panel meetings to give early career researchers insight into how the selection process works and broaden access to ARCHER.

- Training:
  - o In final stages of planning a Software Carpentry course in Manchester aimed at attracting female attendees, jointly organised by ARCHER, SSI and WISE.
  - o Experience gained at "8th European Conference on Python in Science" in Cambridge is being used in design of new Scientific Python course.
  - o Training panel videoconference in October will discuss 2016 training plan.

- Outreach:
  - o The supercomputer demonstrator, 'Wee ARCHIE', and the build-a-supercomputer app 'The ARCHER Challenge' will be launched at SC15 in Austin, Texas.
  - o Diversity in HPC website showcasing the Faces of HPC project and best practise in improving diversity will be launched in December 2015.
  - o Women in HPC will run a 'birds of a feather' session and the third international WHPC workshop at SC15 (Austin, Texas in November).
  - o ARCHER Champions face-to-face meeting will run in February or March depending on core participant availability.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: July 2015, August 2015 and September 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	Jul-15		Aug-15		Sep-15		Q3 2015	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
QE1	100%	-2	100%	-2	100%	-2	100%	-6
QE2	100%	-2	95%	-2	100%	-2	98%	-6
TA1	100%	-1	90%	-1	100%	-1	98%	-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

In August, a single long-standing In-Depth query was closed that had taken longer than 4 months to resolve due the complexity of the issue: extracting more information from the system when a job was killed due to running out of memory (the Cray OOM killer stops jobs before diagnostic information can be collected); this lead to the 95% performance on metric QE2. Also in August, a single Instant Access TA took longer than 10 days to complete due to human error; this lead to the 90% performance on metric TA1.

Of the feedback received on In-Depth queries there were five ratings of "Excellent", two ratings of "Good" and one rating of "Satisfactory".

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	Jul-15		Aug-15		Sep-15		Q3 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	Jul-15	Aug-15	Sep-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	Jul-15	Aug-15	Sep-15	Total	% Total
In-Depth	15	22	9	46	15%
Course Registration	56	66	60	182	60%
Technical Assessment: Grant	15	1	6	22	7%
Technical Assessment: RAP	1	1	10	12	4%
Technical Assessment: Instant	1	7	4	12	4%
Technical Assessment: Leadership	2	1	17	20	7%
Technical Assessment: HEC BioSim	0	1	0	1	0%
eCSE Application	1	1	4	6	2%

8 query feedback responses were received on In-depth queries in the reporting period. This represents a 17% return rate for feedback forms.

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	26	57%
User Programs	2	5%
Compilers and system software	4	9%
Performance and scaling	2	4%
Access to ARCHER	1	2%
Other	11	24%

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.

Q576506, Q573766, Q553178, Q469699, Q401516: Enabling use of STAR-CCM+ on ARCHER

We have had a number of long-standing requests to run the commercial CFD software, STAR-CCM+, on ARCHER from a variety of projects and prospective users. Initially, this was problematic due to the requirement for a license server visible to the compute nodes. The installation of the Cray RSIP service during the Phase 2 upgrade provided the infrastructure required to meet this requirement. CSE collaborated with SP to configure the RSIP service and a FLEXlm license server in such a way that it could be used to supply STAR-CCM+ licenses to the ARCHER compute nodes. Once this work was complete, the CSE team liaised with CD-Adapco (the STAR-CCM+ vendor) to install and test a copy of the software on ARCHER. This was not a straightforward process and involved coordination with Cray, ARCHER systems team and the

external vendor to get to the point of the software working on ARCHER. We are now in the process of agreeing licensing logistics with CD-Adapco before publicising the availability of the software on ARCHER.

Q570634: Trouble linking to NetCDF

A user was having issues building a pre-release version of the WAVEWATCH III software on ARCHER – in particular, in getting the software to link to the NetCDF portable data format libraries. As the software was pre-release, the build process was not mature and well understood. The CSE team was able to analyse this complex build process and provide a solution that allowed the software to be compiled on ARCHER and linked against the requisite libraries. The user was also provided with advice to feedback to the code developers on how they could improve the build process to make it more robust and portable in the future.

Q539371: ADF on ARCHER

The ADF program is currently the only software that supports the Spin Orbit, Time Dependent DFT (SO-TDDFT) method required for a user's research on ARCHER. The ADF developers do not release source code for the program and did not have a recent build of the application for Cray XC architectures. CSE team coordinated with SCM (the developers of the ADF software) to produce a version built for the Cray XC architecture and to get it installed in a central location on ARCHER for all users to access. Once this had been produced the complex set of scripts required to run ADF had to be modified by the CSE team to make them suitable for a Cray XC system rather than a standard HPC cluster. We are following up this installation by benchmarking the ADF code on ARCHER and will provide this information to ARCHER users and feed it back to the ADF developers so that all users of ADF worldwide can benefit.

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 3 weeks (median resolution time since 1 Jan 2014 is 2 weeks).
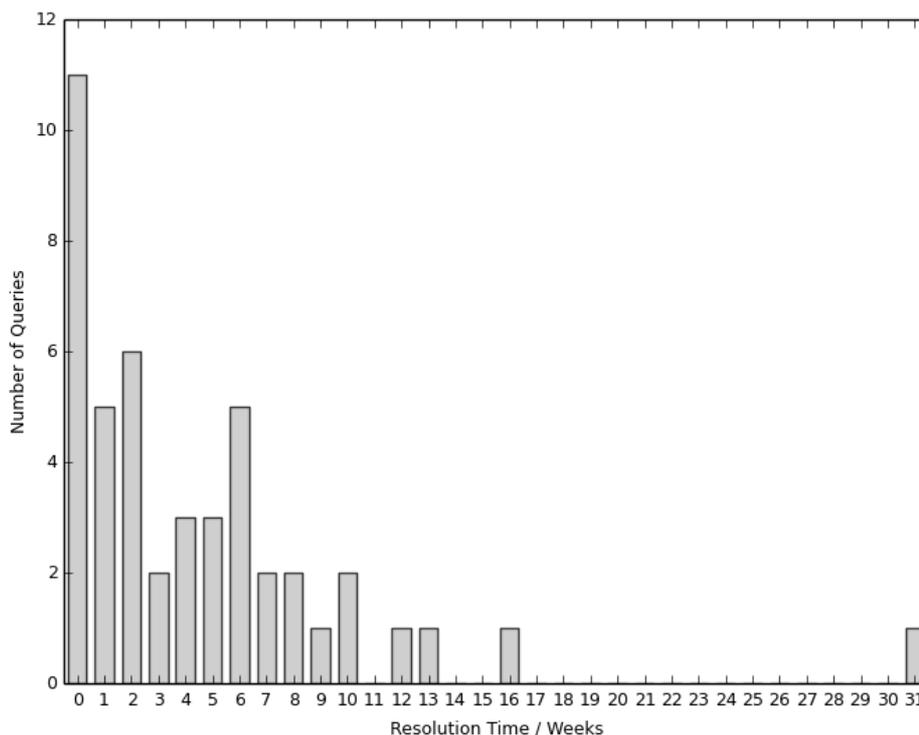
Technical Assessment Completion Times

A histogram of the time to completion for Technical Assessments (see below) reveals that the median completion time for this quarter was 3 days (median completion time since 1 Jan 2014 is 3 days). There were 66 Technical Assessments requested this quarter, compared to 37 in the previous quarter. This increase is due to the RAP and Leadership calls 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
- Q3 2015: 66
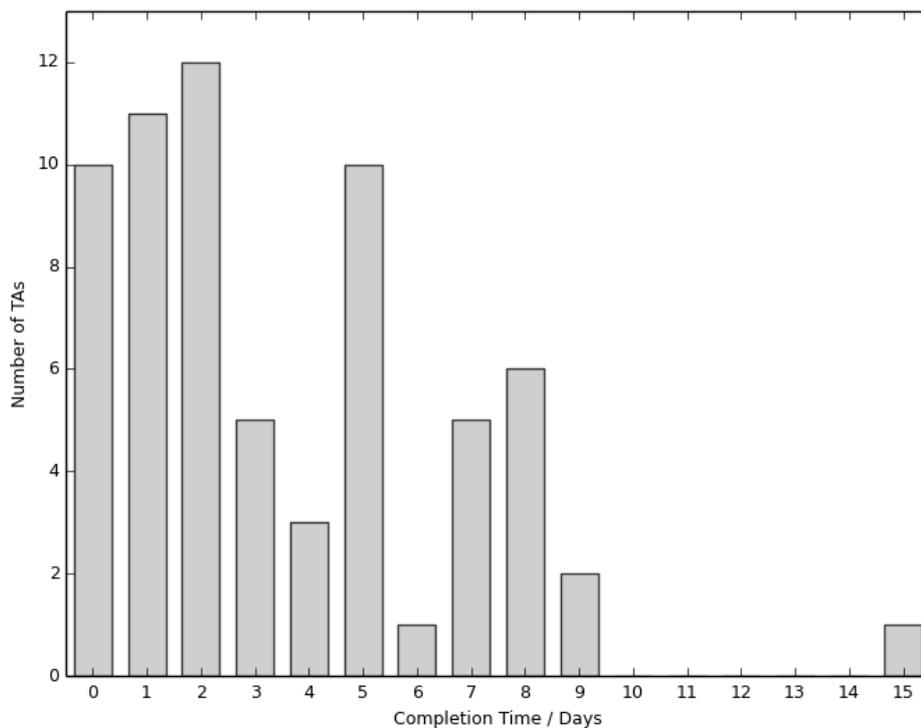
6. Training

The CSE Service has provided a total of 12 days (253 student-days) of face-to-face training across three different locations in the reporting period, plus 2 days of interactive online training.

Month	Dates	Course	Location	Days	Attendees
Jul 2015	2 – 3	Advanced OpenMP	Manchester	2	18
	8	Compilation and the Mysticism of Make	Online	0.5	22
	13 - 14	Hands-on Introduction to HPC	Edinburgh	2	26
	12	Bash is Awesome!	Online	0.5	28
	15 - 17	Message-Passing Programming with MPI	Edinburgh	3	16
Aug 2015	24 - 25	Shared-Memory Programming with OpenMP	London	2	21
	26	Submitting an eCSE proposal	Online	0.5	11
Sep 2015	1 - 3	Message-Passing Programming with MPI	London	3	25
	9	Data Management	Online	0.5	15

The two courses in Edinburgh in July comprised a full week of introductory training badged as the "2015 ARCHER Summer School". This event was successful, although the attendance was not as high as in 2014. Last year we were able to offer travel bursaries to students using additional funding from our PRACE Advanced Training Centre. This was not possible in 2015, but we will look at the possibility of bursaries for the same event in 2016.

Attendance figures for the online virtual tutorials have previously been estimated by looking at how many people were in the virtual room at the midpoint of the training. We have recently instigated a lightweight registration system for these tutorials, meaning we will have more accurate attendance figures in the future. More importantly, attendees can optionally provide their email address. This now enables us to contact them after the event, for example to provide additional information on a question that was raised during the training. We now also provide a feedback button as an easy way for people to report any technical problems.

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 4.5. i.e. better than "Very Good"; users provided 57 feedback forms on the CSE courses, a response rate of 54%.

A total of 21 days of face-to-face training are planned for the next quarter (of which 2 days will also be available online), plus 0.5 days of purely online training. Details are provided below.

Month	Dates	Course	Location	Days	Attendees
Oct 2015	14, 21, 28 & 4 Nov	Scientific Computing	Edinburgh and online	2	
	28 - 29	Advanced MPI	Edinburgh	2	
	29 - 30	Data Carpentry	Leeds	2	
Nov 2015	11	OpenMP 4.0	Online	0.5	
	23 - 24	Scientific Python	London	2	
	24 - 25	Practical Software Development	Edinburgh	2	
	TBC	Software Carpentry	Manchester	2	
Dec 2015	1 -2	Single Node Performance Optimisation	Bristol	2	
	10 – 11	Efficient Parallel IO on ARCHER	Oxford	2	
	15 - 16	Shared-Memory Programming with OpenMP	York	2	
	15 - 16	Software Carpentry	Portsmouth	2	
	17	Introduction to HPC	Portsmouth	1	

Online Training

The "Scientific Computing" course starting in October is being delivered in Edinburgh as four half-day sessions on consecutive Wednesday afternoons. To enable all ARCHER users to benefit from this course it will be available as a live webcast and recorded for the ARCHER website. The extended format will give students a full week between each session to undertake the associated programming exercises. Remote attendees can register in advance to obtain a training account on ARCHER, which will be available to them for the month-long duration of the course.

As well as recording all virtual tutorials and making them available as videos on the website, we are now also able to capture the Q&A chat sessions which take place after any formal presentation. The record of the chat session is made available as a separate document. These documents are a valuable resource as both questions and answers can often include code snippets or web URLs that are best represented as plain text.

7. Outreach Project

Work Package 1: Diversity

Current/completed activities:
- Diversity in HPC website (www.hpc-diversity.ac.uk) – site in development, including a section on best practice and the Faces of HPC project.
  - Website launch planned for 1 December 2015.
- Faces of HPC (Changing the Face of HPC):
  - Eight Interviews with HPC users and three biographies showcasing the work of leading HPC figures have been completed during this reporting period.
  - Continuing programme of interviews over the lifetime of the project, with a minimum of 16 interviews/biographies to go live at launch of the website on 1 December 2015.
  - Faces of HPC project will continue to be developed for the remaining 30 months of the project with an average of 1 new interview/historical biography created per month
- Improving accessibility to training materials
  - Investigation into best practice for providing accommodations for training has begun
  - All ARCHER training courses will now have a separate form after successful registration for participants to provide information on accommodations they need, decoupling the registration procedure from the request for assistance.
  - An ARCHER webinar on best practice in providing accessible training is scheduled for Wednesday 4 November 2015. This material will also be provided as a best practice guide on the Diversity website.
- Women in HPC workshops/training
  - UK (London, September 2015) and European (in collaboration with ISC15, Frankfurt, July 2015) workshops have been completed in this reporting period.
  - 15 attendees from the UK event provided feedback: 10 rated the event as 'Excellent' and 5 as 'Good'.

Future activities:
- Best practice and experience papers – the first best practice guide is scheduled for work in Q4 2015, with additional papers added over the lifetime of the project.
- Series of blog articles – start mid 2016, continue for lifetime of project.
- Women in HPC at SC15: a workshop and BoF will take place at SC15 in November in Austin, Texas.

Work Package 2: User Engagement and Skills Development

Current/Completed activities:
- ARCHER Champions:
  - A teleconference took place where invited participants from representative regional centres and ARCHER staff discussed the format of the ARCHER Champion initiative. The meeting was very positive. We are now planning the first Champions workshop for Q1 2016 based on the outcomes of the teleconference.
  - Jo Beech-Brandt (ARCHER Champions lead) attended the HPC-SIG meeting on 24 September and outlined the brief for the Champions initiative. This was well received by the group and has resulted in a larger group of potential participants for the first face-to-face meeting.

Future activities:
- Future hands-on porting workshops, dates and locations to be decided.

Work Package 3: Outreach programme

Current/Completed activities:
- Wee ARCHIE
  - Wee ARCHIE, the model supercomputer constructed from 18 Raspberry Pi 2s has now been built
  - Two example HPC applications have been ported to the cluster: the Dinosaur racing demonstration using a task farm and a fractal simulation that highlights the issue of optimal load balancing.
  - The official launch of Wee ARCHIE will take place at SC15 in Austin, Texas.
- Design-your-own-supercomputer App: the 'ARCHER Challenge' app has now been completed and tested at various local events
  - Two modes of play are available: independent user who can continue playing the game until they are defeated by the amount of 'incoming work'; and festival mode, used at events to produce a best score in a limited amount of time.
  - Designed for use on a tablet or laptop but, as a web app will also work on all smartphones, it is not limited by platform.
  - Official launch will also take place at SC15 in Austin, Texas.

Future activities:
- National outreach activities designed to reach a wide geographical distribution of schools and children. Two main activities identified:
  - ARCHER will have a booth at the Big Bang Festival at the NEC in Birmingham, 16-19 March 2015. Last years event had over 70,000 children visit across 4 days, primarily from the south of England and midlands.
  - We plan to obtain accreditation from the Children's University for some of our on-line outreach material. This nationwide scheme operates a credit-based passport and should provide benefit to schoolchildren throughout the UK.
- Teacher and Outreach ambassadors pack: work to start Autumn 2015
- Online outreach resources: to be developed alongside the outreach pack (Autumn 2015)
- Teacher support forum and tutorials – 2016/17
- Outreach ambassador training programme – mid 2016.
- Teacher's workshop – mid/late 2016.

Work Package 4: Impact Material

**Current/Completed activities:**
- ARCHER case studies: five completed.
- Impact competition 2015: closed 30 September 2015 next week
  - Close 30 September 2015: unfortunately received only 2 entries.
  - Entries will contribute to the annual impact report
- Image competition 2015
  - Close 30 September 2015: received 30 entries.
  - After the success of the 2015 ARCHER calendar the entries to the image competition will be used to produce a 2016 calendar.

Future activities:
- Annual impact and success report – to be completed in Autumn 2015
- Continuing programme of case study development from eCSEs, image and impact competition, etc.

8. Embedded CSE (eCSE)

Overview of eCSE Effort
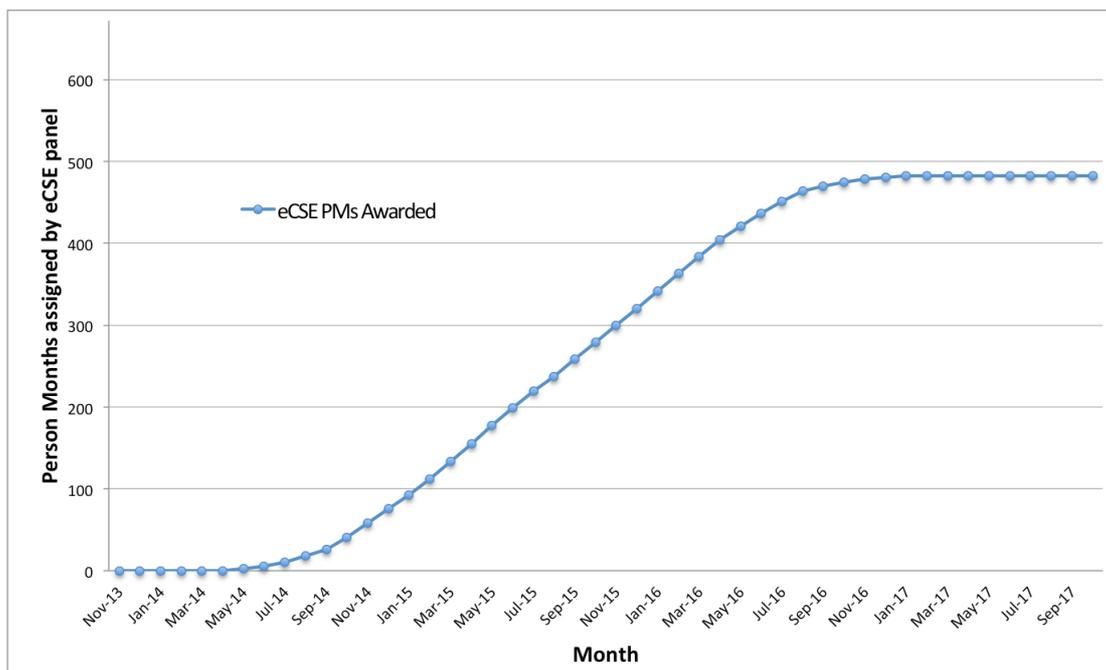
- The eCSE person months awarded up to and including the 5th eCSE call are shown in blue
- At least 672 person months will be awarded by the end of the project (14 FTEs for 4 years)
- 492 person months have been awarded so far over 50 awarded eCSE projects. One eCSE04 project (eCSE04-1) was accepted with the condition that the PI agreed to a reduced number of person months (but with no reduction in the work to be completed). The PI decided to withdraw rather than accept reduced funding meaning that the 6 person months awarded conditionally to this project go back in to the available pool of effort. This leaves 486 person months of effort across 49 projects awarded and expected to complete.

eCSE Call 1

- 12 of the 14 projects have completed with 7 final reports received. The remaining reports for completed projects are due shortly, with one presently overdue; this late report is being pursued.
- A risk analysis identified all projects as being of either low or very low risk apart from eCSE01-019 that was considered to be of medium risk due to difficulties in agreeing staffing for the project.
    o This project is now 60% of the way through and progress is being monitored via the eCSE contact within the centralised CSE team

eCSE Call 2

- 8 of the 9 projects have completed with 3 final reports received. The remaining reports for completed projects are due shortly with one presently overdue; this is being pursued.
- A risk analysis identified all projects as being of either low or very low risk apart from the following:
    o eCSE02-2 which was considered to be of medium risk due to its reliance on outdated versions of OpenFOAM.

- This project had been progressing well but the member of staff working on the project became ill and the project has terminated early.
  - 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.
    - The staffing for this changed for a second time and the activity will now recommence with a member of the UCL Research Software Development group taking on the work from 01/10/15.

eCSE Call 3

- 9 out of the 10 projects have started, 1 has been completed with a final report due shortly
- One project (eCSE03-11) has a delayed start due to the PI moving and staffing changes. This project will start on 01/12/15.
- 6 projects require contracts. 4 have been signed and 2 are 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:
  - 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

- 7 of the 8 projects have started
- 6 projects require contracts; 4 have been signed. The contracts for 2 projects that had staffing changes are 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 project was dependent on this being accepted by the PI.
    - This project has been withdrawn as the PI felt that the reduction in time awarded would not be adequate to complete all of the original aims, the completion of all of which were still required by the panel despite the reduced funding
  - eCSE04-4 which was identified as being of medium risk as the person named to do the technical work was offered a position elsewhere.
    - The member of staff originally named on the contract completed 1.5 of the 12 months of work before leaving to take up another post. We have now identified a new member of staff within the ARCHER CSE team to staff this project from 01/10/15. The PI and Panel chair have approved this arrangement.
  - eCSE04-10 which was identified as being of medium risk as the PI indicated that the person named to do the technical work may not be available.
    - This project will go ahead with the original staffing. There will be a short delay and the project will now start on 01/01/16
  - eCSE04-16 which was identified as being of medium risk as the PI indicated that the person named to do the technical work may not be available.
    - This project will go ahead with a short delay and a change of staffing. This project was originally to be staffed by Imperial College but will now be staffed by STFC. The PI and Panel chair have approved this arrangement.

eCSE Call 5

- 5 of the 8 projects have started.
- 5 projects require contracts. 3 have been signed, 1 is awaiting signature and for 1 project there is a change of staffing to be finalised

eCSE Call 6

- The eCSE06 call opened on 04/08/15 and closed at 4pm on 15/09/15; 9 proposals were received and are presently under review.
- The eCSE06 Panel meeting will take place on 25/11/15
- For the eCSE06 call, updated guidance was provided on filling in the proposal form with regard to finances and staffing as well as other minor updates

Future eCSE Calls

- eCSE calls are run to a regular schedule. The future calls are:
  - 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	finished 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	finished 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 31/07/2015
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	finished 31/01/2015 Final report received
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 31/12/2014 Final report received
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 31/08/2015
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);	12	finished 31/05/2015

			Dr Mayeul d'Avezac (3/UCL)		
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 31/03/2015 Final report received
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 30/11/2014 Final report received
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 30/06/2015 Final report received
eCSE01-017	Dr Matt Probert <matt.probert@york.ac.uk> (York)	*Hybrid OpenMP and MPI within the CASTEP code*	Edward Higgins (12/York)	12	finished 31/05/2015 Final report received
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	started 01/01/2015 finishes 31/03/2016
eCSE01-019	lian Todorov <Ilian.todorov@stfc.ac.uk> (STFC)	*DL_POLY_4: Multiple Time Stepping Development Support*	Ian Bush (6/Oxford)	6	finished 31/08/2015

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	finished 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	finished 30/06/2015 Final report received
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	finished 30/06/2015 Final report received
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	finished 31/08/2015
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 (1.5/UCL); Dr Mayeul d'Avezac (5.25/UCL); Dr Gary Macindoe (5.25/UCL)	12	started 01/02/2015 finishes 31/07/2016
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	finished 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 Final report received

eCSE02-17	Dr James Harle <jdha@noc.ac.uk> (NOC)	NEMO Regional Configuration Toolbox	Srikanth Nagella (6/STFC); Shirley Crompton (3/STFC)	9	finished 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	finished 31/08/2015
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 31/12/2015
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 01/02/2015 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*	Sergey Chulkov (12/UCL)	12	starting 01/12/2015 finishes 30/11/2016
eCSE03-12	Xuerui Mao <xuerui.mao@durham.ac.uk> (Durham)	*Full parallelism of calculations of optimal flow control*	Bofu Wang (12/Durham)	12	started 01/07/2015 finishes 30/06/2016
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*	Derek Groen (2/UCL); Rupert Nash (10/EPCC)	12	started 01/03/2015 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	WITHDRAWN
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 (1.5/Edinburgh (non EPCC)); Kevin Stratford (10.5/EPCC)	12	started 01/04/2015 finishes 31/07/2016
eCSE04-7	Jonathan Essex <jwe1@soton.ac.uk> (Southampton)	*Implementation of Dual Resolution Simulation Methodology in LAMMPS*	Iain Bethune (6/EPCC)	6	started 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 01/01/2016 finishes 31/12/2016
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	finished 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	started 01/08/2015 finishes 31/07/2016

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 01/06/2015 finishes 31/03/2016
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	started 01/09/2015 finishes 30/06/2016

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); Gavin Pringle (2/EPCC)	14	starting 01/10/2015 finishes 30/09/2016
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*	José David Arregui-Mena (6/Manchester); Luis Cebamanos (6/EPCC)	12	starting 01/11/2015 finishes 31/10/2016
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); Jens Hedegaard Nielsoen (9/UCL)	12	started 01/09/2015 finishes 31/05/2016
eCSE05-7	Dr. Angus Creech <a.creech@ed.ac.uk> (University of Edinburgh)	*Optimisation of Large Eddy Simulation (LES) turbulence modelling within Fluidity*	Adrian Jackson (12/EPCC)	12	started 01/08/2015 finishes 31/07/2016
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	starting 01/10/2015 finishes 30/09/2016

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	started 01/09/2015 finishes 30/04/2016
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); Dr Neelofer Bangawala (1/EPCC)	12	started 01/09/2015 finishes 31/07/2016
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); Arno Proeme (2/EPCC)	12	started 01/08/2015 finishes 31/07/2016

eCSE Call 6: Proposal List

eCSE ID	PI (Institution)	Title	Technical Staff (PMs/Institution)	PMs	Status
eCSE06-1	Matthew Piggott <m.d.piggott@imperial.ac.uk> (Imperial College London)	*Integrating mesh movement ("r"-adaptive) technology within Fluidity and the PRAgMaTIc parallel anisotropic ("h") adaptive mesh toolkit*	Tim McManus (12/Imperial College London)	12	01/11/2015
eCSE06-2	Prof Mark Wilson <mark.wilson@durham.ac.uk> ()	*GBMol_DD : A code for Coarse Grained Simulations of Soft Matter Systems*	Dr Fatima Chami (12/Durham University)	12	01/02/2016
eCSE06-3	Dr Alex JW Thom <ajwt3@cam.ac.uk> (University of Cambridge)	*HANDE: Making stochastic quantum chemistry scalable and accessible*	ARCHER CSE (7/EPCC)	7	01/01/2016
eCSE06-4	Pankaj Pankaj <pankaj@ed.ac.uk> (The University of Edinburgh)	*Implementation of generic solving capabilities in ParaFEM*	ARCHER CSE (8/EPCC)	8	01/01/2016

eCSE06-5	Dr Ilian T Todorov <I.T.Todorov@dl.ac.uk> (Daresbury Laboratory)	*SHAPED PARTICLES*	Laurence Julian Ellison (18/STFC)	18	00/01/1900
eCSE06-6	Mr Iain A Bethune <ibethune@epcc.ed.ac.uk> (EPCC)	*CP2K - scalable Density Functional Theory*	ARCHER CSE (12/EPCC)	12	01/04/2016
eCSE06-7	Dr Scott M Woodley <Scott.Woodley@ucl.ac.uk> (UCL)	*Exploring Energy Landscapes via a Client-Server Approach to ARCHER Resources*	Tomas Lazauskas (12/UCL)	12	01/01/2016
eCSE06-8	Peter Jan van Leeuwen <p.j.vanleeuwen@reading.ac.uk> (University of Reading)	*EMPIRE optimization and interfacing*	ARCHER CSE (3/EPCC)	3	01/01/2016
eCSE06-9	Dr Benedict Rogers <Benedict.Rogers@manchester.ac.uk> (University of Manchester)	*Developing Massively Parallel ISPH with Complex Boundary Geometries*	Xiaohu Guo (12/STFC)	12	01/11/2015