ARCHER CSE Service Quarterly Report

Quarter 1 2015

1. Executive Summary

This report covers the period: 1 January 2015 to 31 March 2015 inclusive.

- Centralised CSE Team:
  - o The CSE team resolved 324 queries during this reporting period.
  - o 36 In-Depth queries were received during the quarter. Trends so far indicate that the number of In-Depth queries received each quarter is stabilising to around 30-40 per quarter (roughly one every 3 days).
  - o The median resolution time for In-Depth queries is 4 weeks ensuring resolutions for users in a timescale where the solution is still relevant.
  - o Screencasts on using the CrayPAT profiling tool and running the DDT debugger are available on the ARCHER YouTube channel and we will add further screencasts over the coming months to help users get the most from ARCHER.
- Summary of feedback:
  - o Feedback on query handling uniformly rated the service as "Excellent". The return rate on query feedback forms has dropped below 15% for the first time (the return rate was 6% for this quarter).
- Training:
  - o Provided 12 days (277 student-days) of face-to-face training in the quarter, at 4 different locations, reducing the requirement on attendees to travel large distances.
  - o Provided 1.5 days of virtual tutorials as interactive webinars. All virtual tutorials are now made available on the ARCHER YouTube channel after delivery.
  - o Initial analysis completed of survey measuring longer-term impact of training; summary report circulated to EPSRC and ARCHER Training Panel.
  - o Second training impact survey to be issued at the start of April.
  - o 45 eligible users have successfully completed the online ARCHER Driving Test; of these, 28 now have ARCHER accounts and have used in excess of 4000 kAUs.
  - o Online training material relevant to driving test now includes recordings of three key lectures.
- eCSE:
  - o All 14 projects from the 1st eCSE call and all 9 projects from the 2nd eCSE call have now started. From the 3rd call, 7 of the 10 accepted projects have started.
  - o Final report instructions and templates have been sent out to the 4 completed projects from the 1st call and one such completed report has been received with the others due within the next month.
  - o The 4th eCSE call opened on 25 November 2014 and closed on 13 January 2015; 16 proposals were received, of which 9 were accepted at the panel meeting on 2 March 2015; one of these was accepted conditionally and this is presently under discussion.
  - o For the 4th eCSE call, proposals from New Communities not already exploiting the ARCHER system were encouraged. The proposal form and guidelines were adapted to assist applicants from New Communities. A subset of person months was reserved for proposals from New Communities and these were considered preferentially during the panel meeting, after which any unfunded New Community proposals were ranked against regular proposals. Any unused person months were then put into the pool to be used for regular proposals. Of the 16 proposals received, 7 claimed to be from a New Community; 2 of these were funded.
  - o Interim reports have been collected for running eCSE projects. The first two eCSE webinars took place in January and February:
    - ▪ 28 January 2015 *A Pinch of salt in ONETEP's solvent model* (Lucian Anton, Scientific Computing Department, STFC, Daresbury Laboratory; Jacek Dziedzic, Chris-Kriton Skylaris, School of Chemistry, University of Southampton)
    - ▪ 25 February *2015 Experiences with porting CESM, or the Community Earth System Model, on ARCHER* (Dr Gavin J. Pringle, EPCC)

2. Impact Summary

- Outreach Activities:
  - o Careers Day at Our Dynamic Earth, Edinburgh, 23 March 2015
  - o RSE@Schools, Greenwood Academy, Irvine, 5 March 2015
  - o Portobello High School Careers Convention, Edinburgh, 26 February 2015 (https://www.epcc.ed.ac.uk/blog/2015/03/03/portobello-high-school-careers-convention)
- Meetings Attended by Centralised CSE Team:
  - o UKCTRF Management Committee Meeting, Newcastle, 12 January 2015: provided technical input and discussed training requirements.
  - o EPSRC ARCHER RAP Meeting, Swindon, 30 January 2015: provided technical and system usage advice to panel.
  - o Science for a Successful Nation, London, 2 March 2015: manned ARCHER exhibit and presented its use and impact to attendees.
  - o EPSRC Future of HPC Workshop, Bristol, 19-20 March 2015: participated in discussions about HPC infrastructure in the UK.
  - o EPSRC HEC Consortia Review, Swindon, 26 March 2015: provided technical input to review meeting.
  - o EPSRC/NERC Leadership Call Panel, Swindon, 27 March 2015: provided technical and system usage advice to panel.
- Presentations by Centralised CSE team:
  - o NSCCS User Meeting, Imperial College, 18 February 2015: lightning presentation and poster on ARCHER and engagement with users of this Tier-2 HPC resource.

3. Forward Look

- Online Material and Documentation
    - o Continue to add screencasts covering technical topics on ARCHER including: interpreting profiler output, checking job scripts for errors, understanding the output from the batch scheduler.
    - o Following suggestions from the Annual Survey, the documentation review is underway to continue to improve the quality and consistency of the online documentation. We plan to implement suggested improvements over the coming months.
- Sharing Technical Expertise
    - o Investigating various options for sharing technical experience and knowledge from the ARCHER CSE team out into the UK HPC community. These include: using online services such as StackExchange and engaging through the community of Research Software Engineers (http://www.rse.ac.uk/).
    - o Will use attendance at Cray User Group meeting in Chicago in April to canvas opinion from other sites on successful initiatives they have used. This will result in a report with ideas for implementation on ARCHER.
- White Papers
    - o Continue to produce ARCHER White Papers on technical topics of interest to users. Planned papers include: use of Cray RSIP technology and historical application usage on UK HPC systems.
- Online training
    - o We are enhancing the training provided by the virtual tutorials by having extended sessions running over several weeks, enabling more time for students to absorb the material or to undertake practical exercises in their own time. We have already scheduled two tutorials on Computer Architectures in Q2, and are planning a similar arrangement for a course on Software Revision Control in Q3.
    - o Plans underway for short introductory online course on "Scientific Computing" delivered as four half-day webinars over four weeks, also recorded and made available online. Timing will be decided to be convenient for new CDT students.
- eCSE:
    - o A number of improvements to the SAFE submission system are planned. For example, allowing proposals to be edited by co-proposers, easier linking of technical staff to proposals, and making the panel review form easier to fill in.
- Suggestions from Annual Survey
    - o CSE will assist in implementing relevant suggestions that have been accepted by the service partners.
- Outreach, Diversity and Impact Grant
    - o Hands-on workshop planned for the 20 April, 18 registrations to date.
    - o ARCHER Champion meeting planned for the week beginning the 8 June (final date to be decided).
    - o Women in HPC event planned for the 4 September at the BCS in London.
    - o Work has begun on the "Wee Archie" mini supercomputer demonstrator.

4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: January 2015, February 2015 and March 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	Jan-15		Feb-15		Mar-15		Q1 2015	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
QE1	91%	2	94%	3	100%	-2	94%	3
QE2	100%	-2	100%	-2	90%	-2	94%	-6
TA1	100%	-1	100%	-1	100%	-1	100%	-3
FB1	N/A	0	100%	-2	N/A	0	100%	-2
Total		-1		-2		-5		-8

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

The response within 3 hours was missed for 1 query in each of the first two reporting periods in the quarter due to human error. For the both of these queries, the user received the response in less than 6 hours. Both queries were resolved to user satisfaction within 4 weeks of the helpdesk receiving the query.

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	Jan-15		Feb-15		Mar-15		Q1 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	Jan-15	Feb-15	Mar-15
Total Service Points	-2	-3	-6

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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	Oct-14	Nov-14	Dec-14	Total	% Total
In-Depth	4	11	20	35	10.8%
Course Registration	54	81	65	200	61.7%
Technical Assessment: Grant	5	6	2	13	4.0%
Technical Assessment: RAP	4	2	1	7	2.2%
Technical Assessment: Instant	9	8	5	22	6.8%
Technical Assessment: Leadership	0	40	0	40	12.3%
Technical Assessment: HEC	1	1	0	2	0.6%
eCSE Application	5	0	0	5	1.5%

All of the feedback left by users on queries was rated "Excellent". 2 query feedback responses were received on In-depth queries in the reporting period. This represents a 6% return rate for feedback forms.

Resolved In-Depth queries fell into the following categories:

Category	Number of Queries	% Queries
3rd Party Software	25	71.4%
User Programs	4	11.4%
Compilers and system software	2	5.7%
Porting	2	5.7%
Performance and scaling	1	2.9%
Other	1	2.9%

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.

Q 466253: TAU toolkit

The TAU performance analysis toolkit (http://www.cs.uoregon.edu/research/tau/home.php) is common on many HPC systems and was requested by an industrial user to help in optimizing the performance of their application. The CSE team liaised with the TAU developers to get a version installed that is optimized specifically for the Cray XC architecture and the user verified that it is working well for them. Initial documentation on using the tool has been added to the ARCHER Best Practice Guide with additional resources to follow. As a follow-on action, the CSE team is investigating the use of TAU for profiling mixed Python+Fortran and Python+C/C++ applications; this is not yet working with other tools on the system and we expect it to be a growing requirement from users as the use of Python in HPC increases.

Q469095: MKL-LAPACK

User code uses the Intel Math Kernel Library (MKL) implementation of the LAPACK dense linear algebra routines and was having some difficultly linking their executable against the multithreaded version of the library as the compile options required can be quite complex. The CSE team was able to help the user get these options correct. In doing so the team also noticed a number of problems with the build setup for the application and were able to advise the user on how to improve the sustainability of their software by improving the build process. Finally, some comments on differences of static versus allocatable Fortran arrays were provided to assist the user in understanding other warning and error messages that arose when compiling. As well as helping the user get on with their use of ARCHER we were also able to update the ARCHER documentation on linking against Intel MKL to provide more detailed information and advice for other users so they can help themselves with MKL on ARCHER and other systems.

Q 466893: paraview access via SSH tunnel

User wished to visualize data on ARCHER using paraview (http://www.paraview.org/) with the client running on their desktop and the server on ARCHER – this particular configuration had not been tried before on the system. The CSE team were able to help the user get the correct, complex SSH setup for the process to work allowing them to user the system as they wished. The configuration required is being added to the ARCHER paraview documentation so that all users can benefit from the experience gained during this query. Rather than the particular HPC expertise of the ARCHER CSE team, this query drew on their familiarity with the specifics of the ARCHER system setup that can be quite different from standard clusters that people are used to using.

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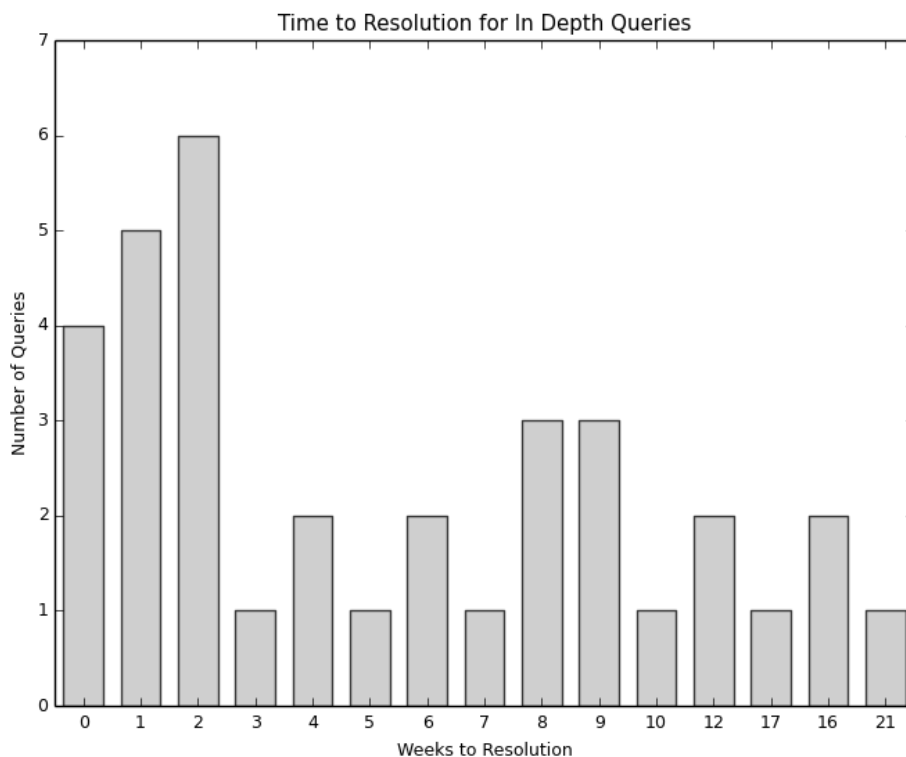
Technical Assessment Completion Times

A histogram of the time to completion for Technical Assessments (see below) reveals that the median completion time for this quarter was 3 days (median completion time since 1 Jan 2014 is 4 days). There were 84 Technical Assessments requested this quarter compared to 38 in the previos quarter. This increase is mostly due to the ARCHER Leadership Call where 40 Technical Assessments were completed by the CSE team. Number of Technical Assessments completed by quarter so far:

- Q1 2014: 23
- Q2 2014: 51
- Q3 2014: 61
- Q4 2014: 38
- Q1 2015: 84
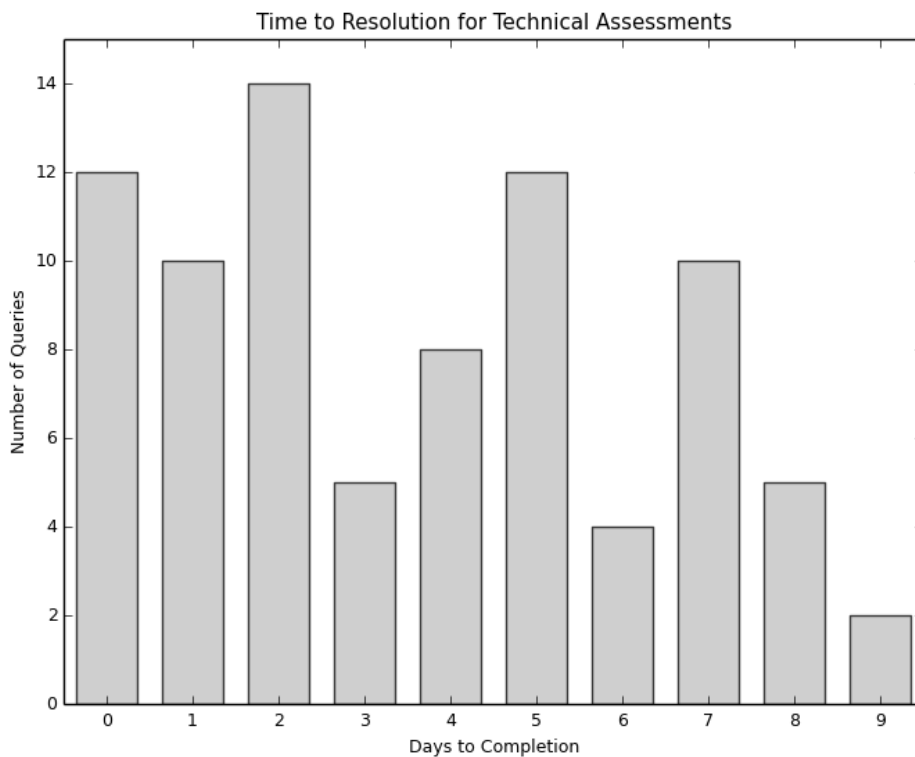
6. Training

The CSE Service has provided a total of 12 days (277 student-days) of face-to-face training across four different locations in the reporting period, plus 1.5 days of interactive web-based training. The table below summarises the training delivered in Q1 2015.

Month	Dates	Course	Location	Days	Attendees
Jan 2015	7	Virtual Tutorial: eCSE Programme Tutorial	Online	0.5	
	28-29	Data Management: IO, Transfer and Storage	Edinburgh	2	21
	28-30	Message Passing Programming with MPI	Sheffield	3	18
Feb 2014	11	Virtual Tutorial: PBS Job Submission	Online	0.5	
	18-19	Fortran 95	London	2	18
Mar 2014	11	Performance analysis on ARCHER using CrayPAT	Online	0.5	
	24-26	Threaded Programming	Southampton	3	33
	30-31	Hands on Introduction to HPC	London	2	23

The "Threaded 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. The same students will also be attending "Message-Passing Programming" in Q2 (see below).

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 4.3. i.e. better than "Very Good". Users provided 56 feedback forms on the CSE courses. This is a response rate of 50%, and we are still receiving feedback for the last two courses in March.
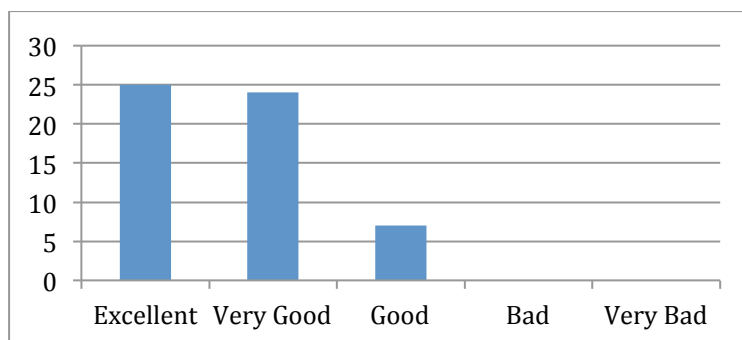

Figure 1: Breakdown of feedback responses from training course surveys for Q1 2015.

A total of 20.5 days of training are currently planned for the next quarter. Details are provided in the table below.

Month	Dates	Course	Location	Days
Apr 2015	8	Virtual Tutorial: Computational Scientist's Guide to Computer Architecture – Part 1	Online	0.5
	15	Virtual Tutorial: Computational Scientist's Guide to Computer Architecture – Part 2	Online	0.5
	14-16	Message-Passing Programming with MPI	Southampton	3
	16-17	Software Carpentry Workshop	London	2
	28-29	Multicore Programming	Edinburgh	2
	30-01	Programming the Xeon Phi	Edinburgh	2
May 2015	5	GPU Programming	Sheffield	1
	7-8	Fortran 95	Oxford	2
	20-21	Single-sided PGAS Communications Libraries	Bristol	2
Jun 2015	10	Virtual Tutorial: Topic TBC	Online	0.5
	25-26	Performance Analysis Workshop	Durham	2
	29-01	Molecular Dynamics Workshop	Glasgow	3

7. Embedded CSE (eCSE)

Overview of eCSE Effort
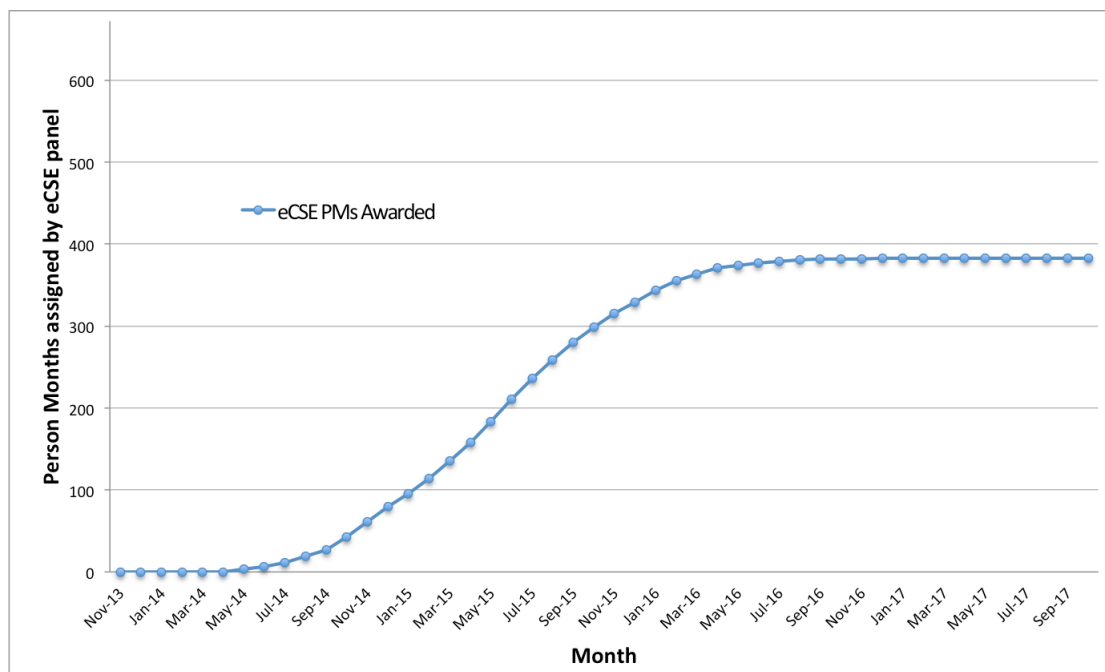
- The eCSE person months awarded up to and including the 4th eCSE call are shown in blue
- At least 672 person months will be awarded by the end of the project (14 FTEs for 4 years)
- 398 person months have been awarded so far over 42 awarded eCSE projects

eCSE Call 1

- All 14 projects have started.
- Contracted being finalised for 1 project.
- 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.
  - o This project has now started and progress will be 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:
  - o 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 have taken place. The project appears to be progressing well.
  - o 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 now started and progress will be monitored via the eCSE contact within the centralised CSE team

eCSE Call 3

- 7 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

- 16 proposals received through SAFE
- 7 proposals claimed they were from New Communities
  - Panel agreed that 3 of them were actually from New Communities, of which 2 were funded
- 9 proposals were successful
- 6 projects require contracts and these 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:
  - 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.
  - eCSE04-4 1 which was identified as being of medium risk as the person named to do the technical work has been offered a position elsewhere. This is being discussed with the PI.

eCSE Call 5

- The 5th eCSE call opened on 31st March and will close on 12th May
- A number of improvements have been 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	started 01/06/2014 finishes 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	started 01/04/2014 finished 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	started 01/06/2014 finishes 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 30/04/2015
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	started 01/09/2014 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	started 01/10/2014 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	starting 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 01/04/2015 finishes 31/03/2016
eCSE03-12	Xuerui Mao <xuerui.mao@durham.ac.uk> (Durham)	*Full parallelism of calculations of optimal flow control*	Bofu Wang (12/Durham)	12	starting June 2015 finishes May 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*	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	starting 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	starting 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 01/05/2015 finishes 30/04/2016

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	starting 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	starting 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 01/05/2015 finishes 31/01/2016