ARCHER CSE Service Quarterly Report

Quarter 1 2014

Summary

This report covers the period: 1 January 2014 to 31 March 2014.

- Given the tight timescales the start of ARCHER CSE Service has progressed extremely smoothly.
- A number of novel engagement initiatives have been put in place to maximize the benefit of the service to users: Consortium Contacts, Technical Forum, Virtual Tutorials.
- Women in HPC initiative initiated to improve the representation of women in HPC and computational science.
- Centralised CSE Team:
    - Centralised CSE team set up including management structure, CSE query, team, training team, eCSE team and consortium contacts.
    - CSE processes based on ITIL best practices for IT services.
    - Close collaborations with Cray Centre of Excellence and Service Desk initiated.
    - 167 queries were resolved by the CSE service during the reporting period.
    - Feedback on query handling from users has been uniformly excellent.
    - ARCHER Best Practice Guide produced and experiences from the service being continually incorporated.
    - Each EPSRC/NERC consortium has a named *Consortium Contact*. An advocate for the consortium in the CSE service and conduit for engagement with the user community.
- Technical Forum:
    - Provides monthly webinars to share experience, knowledge and expertise.
    - Open to all (not just ARCHER users).
    - 3 webinars in reporting period, including presentations by external experts.
    - Also includes a JISCmail list for sharing experience.
- Training:
    - 12 training courses delivered at 6 locations across the UK since the start of the service.
    - Feedback from attendees has been excellent.
    - Content based on experience and curriculum from EPCC's successful MSc in HPC and role as PRACE Advanced Training Centre.
    - 3 virtual tutorials delivered online.
    - Draft curriculum and timetable for 2014 approved by external Training Panel.
    - Further 3 external locations confirmed for courses in Q2 2014.
- Embedded CSE (eCSE):
    - Regular, 4-monthly call schedule put in place.
    - Expert, eCSE panel assembled with representation from all relevant parties.
    - Flexibility of spend profile available to allow funding decisions to be made primarily on quality of proposals.
    - 14 of 19 proposals funded from 1st call. Projects currently in process of starting up.
    - 2nd call is currently open with online submission mechanism through SAFE framework. Make submission simpler for users and processes simpler for reviewers.
    - Improved submission guidance provided based on experience from 1st call.

Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: January 2014, February 2014 and March 2014.

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-14		Feb-14		Mar-14		Q1 2014	
Metric	Perf.	SP	Perf.	SP	Perf.	SP	Perf.	Total
QE1	94%	2	97%	3	100%	-2	97%	3
QE2	100%	-2	100%	-2	100%	-2	100%	-6
TA1	100%	-1	100%	-1	100%	-1	100%	-3
FB1	N/A	0	100%	-2	100%	-2	100%	-4
Total		-1		-2		-7		-10

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

Repeat Failure in metric QE1: missed metric on 2 queries in January 2014, 1 query in February 2014. Additional processes and SAFE functionality have been put in place to help and lead to the steady improvement in performance.

Training Metrics

- **FB2:** The percentage of all training satisfaction 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-14		Feb-14		Mar-14		Q1 2014	
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

CSE Queries

Queries Resolved in Reporting Period

A total of 167 queries were resolved by the CSE service in the reporting period.

Metric	Jan 2014	Feb 2014	Mar 2014	Total	% Total
In-depth	11	51	35	97	58.1%
Course Registration	16	3	14	33	19.8%
Technical Assessment	9	10	4	23	13.8%
eCSE Application	7	2	5	14	8.4%

All of the feedback left by users on queries was rated "Excellent" and comments generally identified the prompt response to support requests. 15 query feedback responses were received in the reporting period.

Resolved In Depth queries fell into the following categories:

Category	Queries	% Queries
3rd Party Software	54	55.7%
User programs	14	14.4%
Compilers and system software	12	12.4%
Batch system and queues	6	6.2%
Disk, tapes, resources	3	3.1%
Performance and scaling	3	3.1%
Access to ARCHER	2	2.1%
Porting	2	2.1%
Courses	1	1.0%

Training

The CSE has provided a total of 18.5 days (249 student-days) of training across 6 different location since the start of the service. The table below summarises the training delivered up until 31 March 2014.

Month	Dates	Course	Location	Days	Attendees
Nov 2013	25-26	Intro to ARCHER	EPCC	2	15
Dec 2013	11	Intro to ARCHER	London	1	30
	16-17	Intro to ARCHER	Daresbury	2	14
Jan 2014	8-9	Intro to ARCHER	Bristol	2	9
	22	Virtual tutorial	Online	0.5	
	28-29	Cray Tools Workshop	EPCC	2	13
Feb 2014	10-11	Intro to ARCHER	Leeds	2	20
	19	Virtual tutorial	Online	0.5	
	25-26	Data Staging & Movement	EPCC	2	3
Mar 2014	3-4	Intro to ARCHER	Belfast	2	21
	12	Virtual tutorial	Online	0.5	
	17-18	PGAS Libraries	EPCC	2	15

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 4.25, i.e. better than "Very good". Users provided 40 feedback forms on the CSE courses.

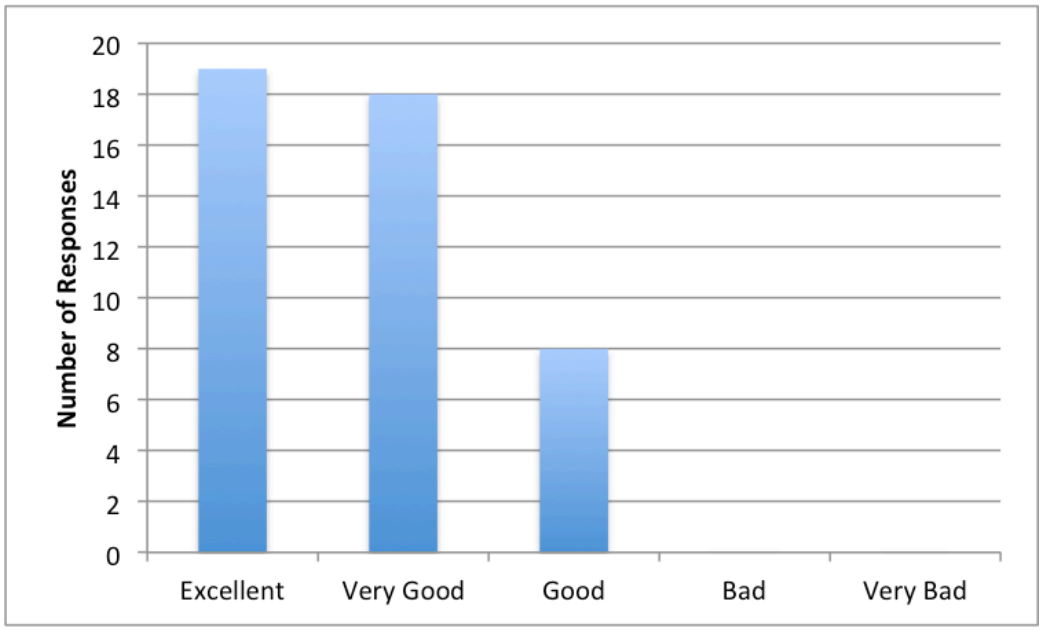

Figure 1: Breakdown of feedback responses from training course surveys for Q1 2014.

22.5 days of training are currently planned for the following quarter. Details are provided in the table below.

Month	Dates	Course	Location	Days
Apr 2014	9-11	Intro to HPC and ARCHER	York	3
	16	Virtual Tutorial	Online	0.5
	23-25	Parallel Materials Modeling Packages	London	3
	23-24	Intro to HPC and ARCHER	EPCC	2
May 2014	29-1	Tools for Large-Scale Parallel Debugging and Profiling	EPCC	3
	6-8	Advanced OpenMP	Oxford	3
	12-13	Introduction to F95	Daresbury	2
	14	Virtual Tutorial	Online	0.5
	29-30	Statistical Analysis for Post-Genomic Data: Parallel Computing with R	Swansea	2
Jun 2014	4-5	Programming the Xeon Phi	Bristol	2
	11	Virtual Tutorial	Online	0.5
Jul 2014	30-4	ARCHER Summer School	EPCC	5

Embedded CSE (eCSE)

eCSE Call 1

- Call Open: November 2013
- Call Deadline: January 2014
- 19 Proposals received (197 months of staff effort)
- 14 Proposals funded (130 months staff effort)
- Projects starting in April and May

eCSE ID	PI	Title	PMs
eCSE01-001	Michail Stamatakis, UCL	Zacros Software Package Development: Pushing the Frontiers of Kinetic Monte Carlo Simulation in Catalysis	12
eCSE01-002	Dr Alan Gray, Edinburgh	Introducing Thread and Instruction Level Parallelism into Ludwig	12
eCSE01-003	Dr Benedict Rogers, Manchester	Developing highly scalable 3-D incompressible SPH	12
eCSE01-004	Chris-Kriton Skylaris, Southampton	A pinch of salt in ONETEP's solvent model	3
eCSE01-005	Mark van Schilfgaarde, KCL	QuasiParticle Self-Consistent *GW* calculations of many-atom systems	6
eCSE01-008	Dr. Prashant Valluri, Edinburgh	TPLS: Optimised Parallel I/O and Visualisation	8
eCSE01-009	Dr Gerard Gorman, Imperial	Scalable and interoperable I/O for Fluidity	6
eCSE01-010	Dr Miguel O. Bernabeu, UCL	Adding a resolved deformable particle model to a highly-parallel blood flow solver for sparse vascular networks	12
eCSE01-013	Jimena Gorfinkiel, Open University	Efficient computation of two-electron integrals in a mixed Gaussian/B-spline basis.	12
eCSE01-015	Professor Michael J Fagan, Hull	Large scale voxel based modelling	15
eCSE01-016	Dr Massimo Bollasina, Edinburgh	Porting and enabling use of the Community Earth System Model on ARCHER	4
eCSE01-017	Dr Matt Probert, York	Hybrid OpenMP and MPI within the CASTEP code	12
eCSE01-018	Scott M. Woodley, UCL	Tuning FHI-Aims for complex simulations on CRAY HPC platforms	12
eCSE01-019	lian Todorov,STFC Daresbury	DL_POLY_4: Multiple Time Stepping Development Support	6

Future eCSE Calls

We plan to run the eCSE calls to a regular schedule. The upcoming calls are:

- eCSE Call 2: Opens 1 Apr 2014, Closes 13 May 2014
- eCSE Call 3: Opens 5 Aug 2014, Closes 16 Sep 2014
- eCSE Call 4: Opens 25 Nov 2014, Closes 13 Jan 2015

Applications to these calls will be through the SAFE web interface.