HECToR Quarterly Report

Jan 2013 – Mar 2013

1 Introduction

This report covers the period from 1 January 2013 at 0800 to 1 April 2013 at 0800.

Section 3 summarises service availability and performance statistics for this quarter. Utilisation statistics are also available in Section 3. A summary table of the key performance metrics is included. Section 4 shows Helpdesk statistics.

The Appendices define some of the terminology and incident severity levels and list the current HECToR projects together with their overall utilisation profile to date.

This report and the additional SAFE report are available to view online at http://www.hector.ac.uk/about-us/reports/quarterly/1Q13.php

2 Executive Summary

- XE6 utilisation in 1Q13 was 79.9% compared to 69.6% in 4Q12. This equates to 99.9% of the optimum 80%. Further details are available in Section 3.2 of the report.

- There was one service failure in 1Q13, which was filesystem related. The overall MTBF improved from 1098 hours in 4Q12 to 2196 hours.

- The volume of single node failures remains low.

- The initial 6 month trial of 24-hour queues ended successfully in 1Q12. The 24-hour queues are now part of the service. Jobs in these queues accounted for 17.1% of the utilisation in the quarter.

- The low priority queue configuration was adjusted in February to enable smaller jobs to run. Low priority jobs accounted for 5.1% of the utilisation in 1Q13. Further details are available in Section 3.2.

- Reservations continued to prove invaluable not only for training courses, but also for supporting users' urgent computing needs. One such example was in support of an article published in the February 2013 edition of' 'New Scientist' magazine.

- The helpdesk statistics were excellent. Positive quality tokens were received from users and there were no negative tokens. Further details are in Section 3.

- 1Q13 saw a reduction in the amount of planned system downtime, with a number of 'At-Risk' maintenance sessions being run

- Work will commence in 2Q13 to investigate the options available for relocating existing user data from the Archive to the RDF. Three "Data Mover Nodes" were configured on the RDF in 1Q13. These enable users to transfer data on/off the RDF to their home institution without the need to login to HECToR. Additional services can be configured on these nodes as required in order to aid the data transfer process.

- The HECToR GPU was restored to service in 1Q13 following a full rebuild after a hardware failure. A small number of users continue to use the system.

3 Quantitative Metrics

3.1 Reliability

The monthly numbers of incidents and failures (SEV 1 incidents) are shown in the table below:

	Jan	Feb	Mar
Incidents	10	17	11
Failures	1	0	0

3.1.1 Performance Statistics

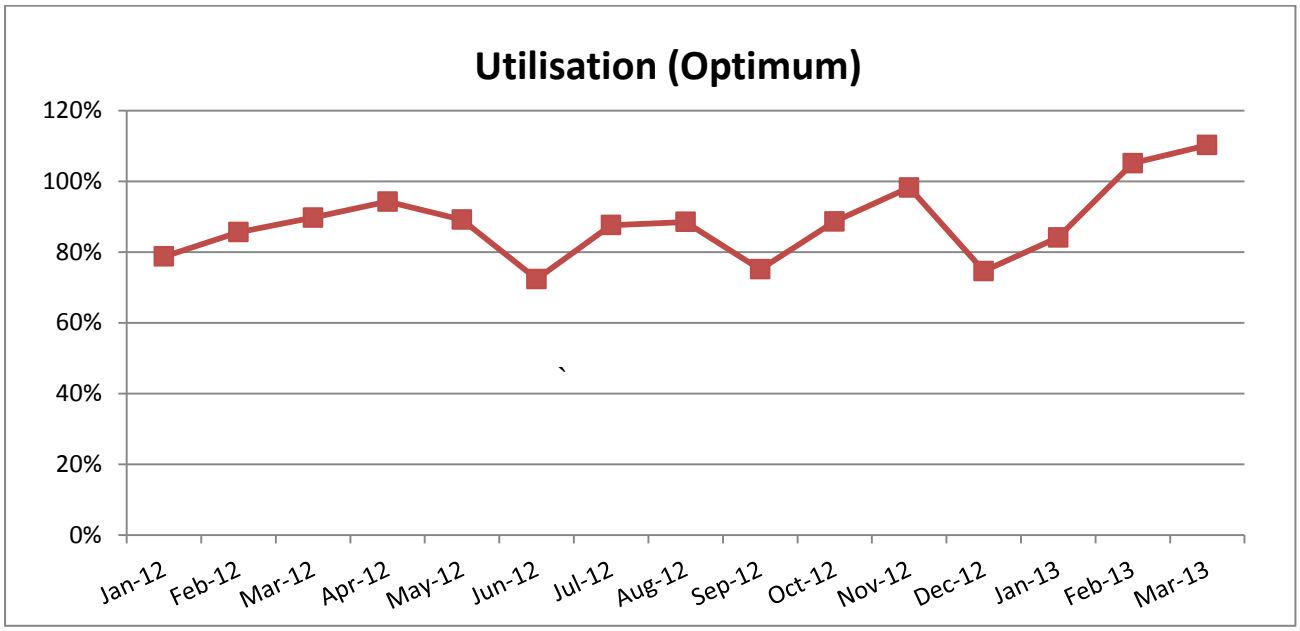
MTBF = (732)/(number of failures in a month)

Quarterly MTBF = (3x732)/(number of failures in a quarter)

Attribution	Metric	Jan	Feb	Mar	Quarterly
Technology	Failures	1	0	0	1
	MTBF	732	∞	∞	2196
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	1	0	0	1
	MTBF	732	∞	∞	2196

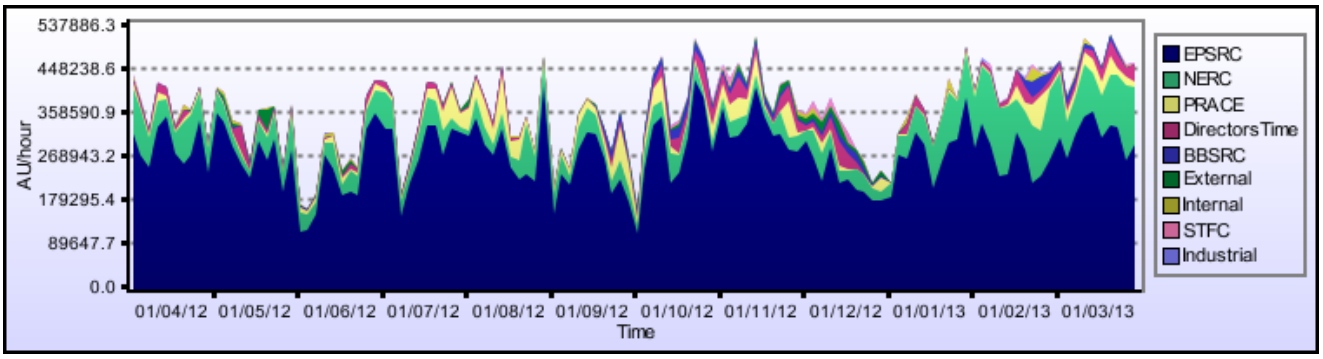
3.2 HECToR Utilisation

3.2.1 XE6 Utilisation



The XE6 utilisation quarterly average in 1Q13 was 99.9% of optimum, compared to 87% in 4Q12.

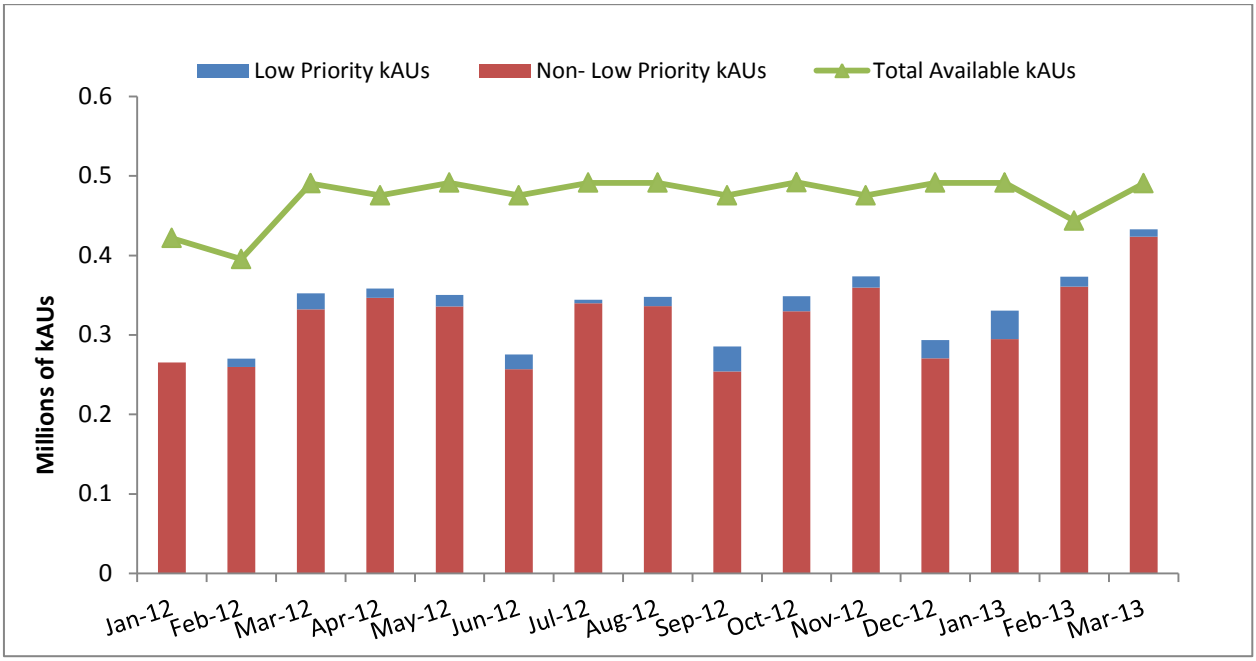
3.2.2 Capability Usage



Raw AUs used by Funding Body of jobs using more than 511 CPUs

3.2.3 Low Priority Access

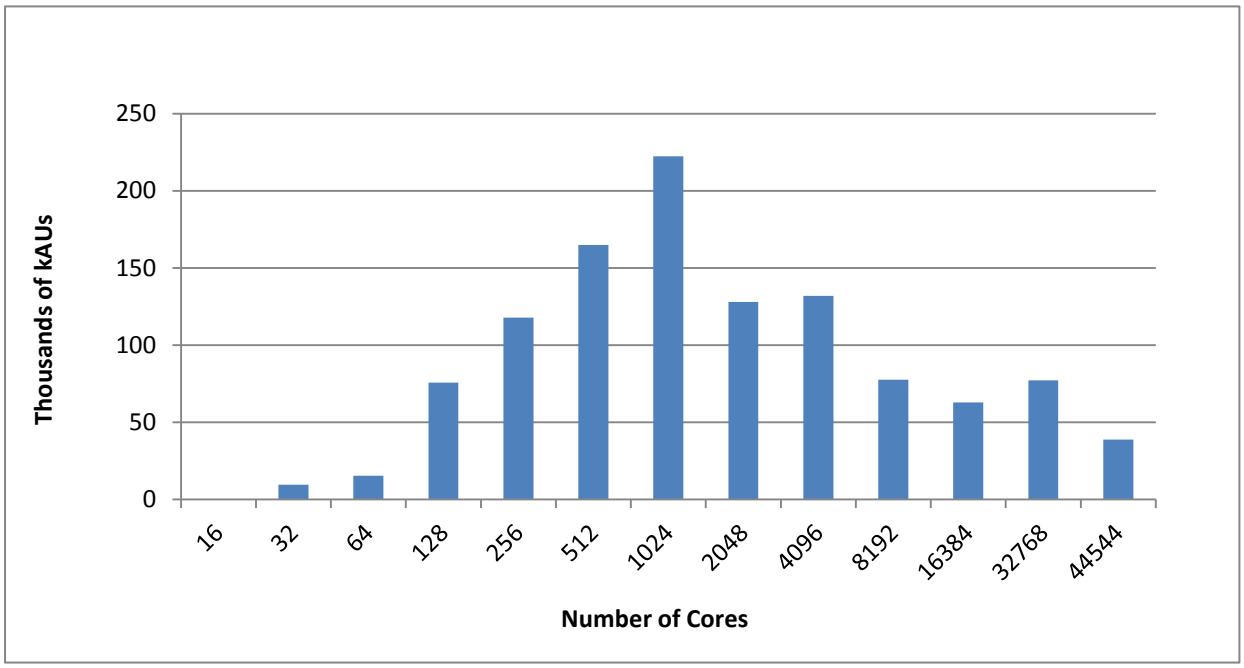
In 1Q13, low priority access accounted for 5.1% the overall utilisation.



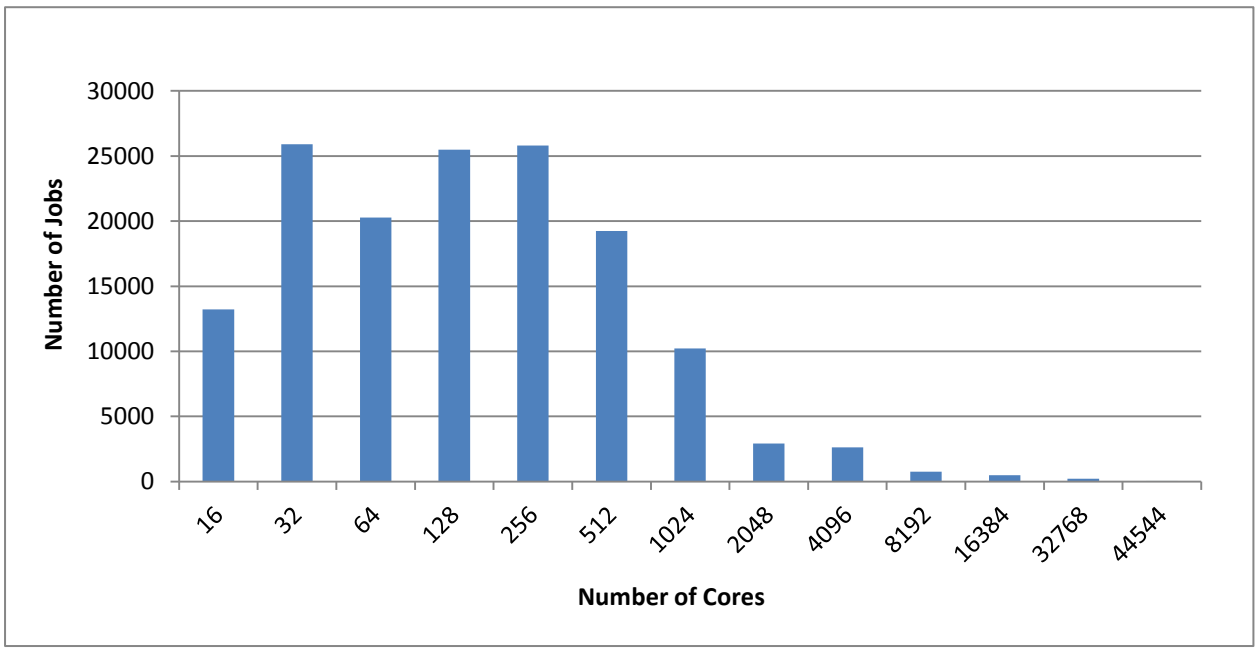
The low priority queue configuration was adjusted in February to enable smaller jobs to run. The lower limit for low priority jobs was reduced from 4096 cores (128 nodes) to 512 cores (16 nodes) at the request for the HECToR Strategic Management Board.

The low priority queues are only enabled when the paid backlog on the system is low, or in the run up to maintenance sessions. The utilisation of the service has been at such a level in February and March that the low priority queues have rarely been enabled.

3.2.4 Utilisation by Core Count



3.2.5 Number of Jobs by Core Count



3.2.6 Utilisation by Consortium

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
y02	0.0	0.0	3	0.0%
y03	610.1	702.8	3,195	0.1%
y04	1.5	2.5	22	0.0%
y07	0.4	0.8	46	0.0%
z01	955.8	1636.2	1,629	0.1%
z03	3261.3	5828.2	1,026	0.4%
z06	0.1	0.2	1	0.0%
Internal Total	**4829.3**	**8170.8**	**5,922**	**0.6%**
c01	1216.5	2136.6	1,780	0.2%
e01	25816.9	67193.1	6,373	4.7%
e05	139577.6	261621.9	24,494	18.4%
e10	6330.5	11416.4	1,433	0.8%
e42	0.0	0.0	4	0.0%
e68	0.2	0.4	3	0.0%
e71	6856.1	11737.3	782	0.8%
e72	0.0	0.0	1	0.0%
e82	647.5	1108.5	29	0.1%
e89	32450.9	70236.1	10,535	4.9%
e104	821.4	1410.0	322	0.1%
e107	123.4	1250.8	118	0.1%
e108	8262.7	14144.9	508	1.0%
e110	14578.0	26453.0	896	1.9%
e122	19417.0	33285.6	3,174	2.3%
e124	0.0	0.0	7	0.0%
e125	2698.7	4619.9	292	0.3%
e126	3652.7	6253.0	64	0.4%
e127	260.3	445.6	7	0.0%
e130	26.7	45.7	27	0.0%
e141	392.2	671.5	254	0.1%
e142	0.0	0.0	20	0.0%
e145	3.1	5.3	4	0.0%
e149	4472.2	7657.2	143	0.5%
e155	1218.4	2085.8	59	0.2%
e158	172.5	412.2	39	0.0%
e159	13.9	23.8	274	0.0%
e160	1029.5	1762.4	484	0.1%
e174	353.6	605.3	52	0.0%
e175	4366.2	19838.6	557	1.4%
e179	134.1	229.6	28	0.0%
e182	0.1	0.2	86	0.0%
e183	1801.1	3083.3	34	0.2%
e184	278.3	476.6	236	0.0%
e185	2035.5	3484.6	96	0.2%
e186	8205.9	14472.6	1,185	1.0%
e187	381.2	652.7	655	0.1%
e192	4845.9	8295.7	356	0.6%
e202	9518.5	17092.1	357	1.2%
e203	0.3	0.5	3	0.0%
e204	1272.2	2179.5	223	0.2%
e207	3765.9	16190.6	18	1.1%
e213	12.3	21.1	26	0.0%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
e215	0.0	0.0	1	0.0%
e228	0.6	0.9	6	0.0%
e229	1230.5	2107.5	4,056	0.2%
e231	363.9	622.9	302	0.0%
e235	615.7	1054.6	731	0.1%
e240	10.4	17.8	140	0.0%
e245	43.6	74.6	34	0.0%
e248	3.6	6.1	51	0.0%
e249	22.9	39.3	17	0.0%
e251	0.0	0.0	1	0.0%
e254	4379.9	13749.7	474	1.0%
e256	0.8	1.4	22	0.0%
e257	605.8	1037.1	56	0.1%
e258	2055.2	3518.3	24	0.3%
e259	17094.7	58654.8	116	4.1%
e260	816.7	1398.1	1,113	0.1%
e261	45.0	114.2	81	0.0%
e262	2.0	3.5	31	0.0%
e263	16149.5	27646.2	854	1.9%
e264	95.9	164.2	3	0.0%
e266	1076.9	1845.7	268	0.1%
e269	0.0	0.0	17	0.0%
e271	36.7	109.0	13	0.0%
e272	699.9	1198.2	28	0.1%
e273	160.9	275.4	224	0.0%
e274	279.2	478.0	114	0.0%
e275	125.9	215.5	141	0.0%
e276	277.8	475.5	168	0.0%
e277	17.2	31.6	78	0.0%
e278	166.3	286.9	35	0.0%
j01	230.5	689.1	94	0.1%
EPSRC Total	**353618.1**	**728415.9**	**65,331**	**51.1%**
n01	31392.0	53808.3	9,464	3.8%
n02	68298.5	117774.8	36,016	8.3%
n03	58843.9	100862.8	14,698	7.1%
n04	24320.8	42393.9	6,087	3.0%
NERC Total	**182855.2**	**314839.8**	**66,265**	**22.1%**
b14	6629.0	11348.1	546	0.8%
b15	6.7	11.4	52	0.0%
BBSRC Total	**6635.6**	**11359.5**	**598**	**0.8%**
p01	2167.4	3723.0	180	0.3%
STFC Total	**2167.4**	**3723.0**	**180**	**0.3%**
x01	226.3	387.5	296	0.0%
External Total	**226.3**	**387.5**	**296**	**0.0%**
b10	1.9	3.2	28	0.0%
d11	73.2	190.2	269	0.0%
d15	4.6	7.9	178	0.0%
d25	2279.9	3902.9	364	0.3%
d26	128.1	146.3	1,317	0.0%
d29	152.5	349.4	260	0.0%
d32	47.5	81.4	58	0.0%
d34	0.0	0.0	2	0.0%
d37	3329.5	9582.0	725	0.7%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
d40	48.7	83.3	99	0.0%
d41	6345.1	10862.2	1,823	0.8%
d43	3465.5	5932.7	547	0.4%
d45	32.1	40.6	1,126	0.0%
d49	0.3	0.5	5	0.0%
Directors Time Total	**15908.9**	**31182.5**	**6,801**	**2.2%**
pr1u0002	0.0	0.0	4	0.0%
pr1u0702	7262.5	12442.0	325	0.9%
pr1u0804	0.0	0.0	2	0.0%
pr1u0806	2747.4	4703.3	99	0.3%
pr1u0807	4971.4	8510.5	381	0.6%
pr1u0902	2935.4	5025.0	101	0.4%
pr1u0903	0.9	1.6	142	0.0%
pr1u0904	3365.2	5760.9	123	0.4%
pr1u0905	153.8	263.2	253	0.0%
pr1u0906	0.0	0.0	6	0.0%
pr1u0907	607.7	1040.3	22	0.1%
PRACE Total	**22044.4**	**37746.9**	**1,458**	**2.7%**
i02	88.0	150.9	349	0.0%
i03	8.2	14.1	59	0.0%
i04	52.1	93.5	29	0.0%
i05	165.3	303.8	19	0.0%
Industrial Total	**313.6**	**562.3**	**456**	**0.0%**
Total	**588598.8**	**1136388.3**	**147,307**	**79.7%**

3.3 Helpdesk

A total of 1167 queries with a specified service metric, and 120 queries with no metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	992	1007	98.5%	97.0%
Admin queries finished in 1 day	952	967	98.4%	97.0%
Queries assigned in 30 min	1165	1167	99.8%	97.0%
Technical assessments in 10 days	27	27	100.0%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	682	58.4%
Admin	285	24.4%
In-depth	133	11.4%
Technical	40	3.4%
Technical Assessment	27	2.3%

Queries by Category

Query Category	Queries	Percentage
New User	154	13.2%
Set user quotas	137	11.7%
New Password	135	11.6%
Set group quotas	94	8.1%
None	70	6.0%
Access to HECToR	64	5.5%
Compilers and system software	54	4.6%
3rd Party Software	52	4.5%
Remove account	47	4.0%
Disk, tapes, resources	43	3.7%
User behaviour	35	3.0%
Batch system and queues	34	2.9%
Login, passwords and ssh	28	2.4%
Other	24	2.1%
User programs	20	1.7%
New Group	20	1.7%
Join Project	18	1.5%
Add to group	18	1.5%
Make Reservation	17	1.5%
Static website	14	1.2%
Update account	13	1.1%
Create certificate	13	1.1%
Courses	13	1.1%
SAFE	11	0.9%
Delete from project	11	0.9%
Node Failure	8	0.7%
Performance and scaling	4	0.3%
Delete Certificate	4	0.3%
GPU	3	0.3%
Network	3	0.3%
Grid	2	0.2%
Archive	2	0.2%
Porting	1	0.1%
Delete from group	1	0.1%

Queries by Handler Category

Handlers	Admin	Technical	Technical Assessment	Automatic	In-depth	Total	%age
USL	234	27	0		42	303	35.1%
CSE	4		27		73	104	12.0%
OSG	43	6	0	682	3	734	85.0%
Cray	4	7	0		15	26	3.0%

3.3.1 Quality Tokens

Eight positive quality tokens were received in 1Q13. There were no negative tokens.

Project	Positive Tokens	Comments
d45	* * * *	No comment received
e277	* * * *	No comment received

3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Jan-13	Feb-13	Mar-13	1Q13
Technology Reliability (%)	85.00%	98.50%	99.6%	100.0%	100.0%	99.9%
Technology MTBF (hours)	100	126.4	732	∞	∞	2196
Technology Throughput, hours/year	7000	8367	8705	8746	8690	8714
Capability jobs completion rate	70%	90%	100.0%	100.0%	98.9%	99.6%
Non in-depth queries resolved within 1 day (%)	85%	97%	98.1%	98.4%	99.0%	98.5%
Number of SP FTEs	7.3	8.0	8.0	8.4	8.1	8.2
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

Appendix A: Terminology

TSL : Threshold Service Level

FSL : Full Service Level

SDT : Scheduled Down Time

UDT : Unscheduled Down Time

WCT : Wall Clock Time

MTBF : Mean Time Between Failures = 732/Number of Failures

SP : Service Provision

SP Serviceability% = 100*(WCT-SDT-UDT(SP))/(WCT-SDT)

Technology Reliability % = 100*(1-(UDT(Technology)/(WCT-SDT))

Incident Severity Levels

SEV 1 — anything that comprises a FAILURE as defined in the contract with EPSRC.

SEV 2 — NON-FATAL incidents that typically cause immediate termination of a user application, but not the entire user service.

The service may be so degraded (or liable to collapse completely) that a controlled, but unplanned (and often very short-notice) shutdown is required or unplanned downtime subsequent to the next planned reload is necessary.

This category includes unrecovered disc errors where damage to file systems may occur if the service was allowed to continue in operation; incidents when although the service can continue in operation in a degraded state until the next reload, downtime at less than 24 hours notice is required to fix or investigate the problem; and incidents whereby the throughput of user work is affected (typically by the unrecovered disabling of a portion of the system) even though no subsequent unplanned downtime results.

SEV 3 — NON-FATAL incidents that typically cause immediate termination of a user application, but the service is able to continue in operation until the next planned reload or re-configuration.

SEV 4 — NON-FATAL recoverable incidents that typically include the loss of a storage device, or a peripheral component, but the service is able to continue in operation largely unaffected, and typically the component may be replaced without any future loss of service.

Appendix B: Projects on HECToR

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
EPSRC Projects							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Adrian Wander	113,303.7	54,907.8	58,395.9
e01	UK Turbulence Consortium	EPSRC	Class1a	Prof Richard D Sandberg	2,319,369.9	193,804.1	2,125,565.7
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	6,319,874.0	1,124,664.1	5,195,149.9
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257,748.2	30,636.2	226,969.6
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000.0	49,887.8	112.2
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403.5	65,667.3	64,724.5
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521.8	40,897.9	1,623.9
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	4,853.4	4,801.3	52.1
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088.6	6,285.6	1,803.0
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	2,403,144.5	408,180.7	1,994,963.8
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400.0	13,134.1	17,262.2
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1a	Dr Andreas M Kempf	1,300.0	297.3	1,002.7
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1a	Prof Kai Luo	3,650.0	3,430.8	219.2
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000.0	1,899.4	4,100.6

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e108	Jet Flap Noise	EPSRC	Class1a	Dr Sergey Karabasov	69,284.5	63,230.4	6,054.1
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	156,110.3	119,289.3	36,821.0
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	150,000.0	103,699.7	46,300.3
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168,324.8	41,765.9	126,449.0
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584.0	21,173.2	4,410.8
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000.0	4,414.4	2,585.6
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7,092.1	6,691.8	400.4
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500.0	2,627.1	4,872.9
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350.0	7,849.3	8,500.7
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191.9	499.5	689.9
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082.5	56,061.5	12,021.0
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000.0	1,526.6	8,473.4
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600.0	402.6	1,197.4
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	2,500.0	1,078.2	1,421.8
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3,816.0	63.1	3,752.9
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208.1	17,012.8	3,195.3
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69,895.5	0.0	69,895.5

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4,872.0	0.0	4,872.0
e174	3D instabilities in two-layer flows	EPSRC	Class1b	Dr Prashant Valluri	11,495.4	4,530.9	6,964.4
e175	Fine-Scale Turbulence	EPSRC	Class1a	Prof Richard D Sandberg	50,000.0	13,234.1	36,610.3
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000.0	3,223.1	83,776.9
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8,150.2	0.3	8,149.9
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130,500.0	1,758.3	128,741.7
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000.0	8,266.8	331,733.2
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70,000.0	69,765.7	234.3
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030.2	1,039.4	4,990.8
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40,500.0	4,413.1	36,086.9
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38,345.0	23,967.4	14,377.6
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim N. Biktashev	4,499.6	4,201.9	297.7
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5,000.0	3,361.5	1,638.5
e206	FLAME Agent-Based Simulation Framework	EPSRC	Class1a	Prof Christopher Greenough	410.0	0.5	409.5
e207	Developing DL_POLY Molecular Dynamics Simulation code	EPSRC	Class1a	Dr Kostya Trachenko	25,857.6	24,103.3	1,754.4
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400.0	22.1	377.9
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26,121.6	17,021.6	9,100.0

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e223	Numerical modelling of aorta dissection	EPSRC	Class2a	Prof. Xiaoyu Luo	300.0	0.0	300.0
e226	Novel Vibrational Spectroscopic Techniques	EPSRC	Class1a	Dr Andrew D Burnett	1,032.3	0.0	1,032.3
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50.0	46.4	3.6
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	20,218.3	701.6	19,516.7
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50,000.0	12,598.2	37,401.8
e231	Rapid Alloy Solidification	EPSRC	Class1b	Prof Peter Jimack	5,130.0	1,144.6	3,985.4
e235	Modelling offshore wind	EPSRC	Class1b	Prof Simon Watson	2,100.0	1,231.0	869.0
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400.0	399.0	1.0
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800.0	324.5	475.5
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500.0	1.4	498.6
e242	Study of the Green Fluorescent Protein Fluorophore	EPSRC	Class2a	Dr Garth Jones	400.0	0.0	400.0
e243	Tailored Structures for Orthopaedic Implantations	EPSRC	Class2a	Dr Carmen Torres-Sanchez	400.0	0.0	400.0
e244	VOX-FE: Large Scale FE Bone Modelling on HECToR	EPSRC	Class2b	Prof Michael Fagan	800.0	8.4	791.6
e246	Numerical simulation of capillary blood flow	EPSRC	Class2a	Dr Ellak Somfai	400.0	0.0	400.0
e247	Tool development for multiscale protein folding simulations	EPSRC	Class2a	Dr Robert Best	400.0	220.9	179.1
e248	Testing of a Distributed Coordinate Descent Method	EPSRC	Class2a	Dr Peter Richtarik	400.0	106.3	293.7
e249	Feedback flow control for reducing the aerodynamic drag	EPSRC	Class1b	Dr Aimee Morgans	9,860.0	2,961.1	6,898.9

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e254	Ceramic Composites for Fusion Power	EPSRC	Class1b	Prof Sergei Dudarev	8,371.0	5,509.5	2,861.5
e255	Turbulent Drag Reduction	EPSRC	Class2a	Dr Pierre Ricco	400.0	0.0	400.0
e256	Hybrid simulation on heat transfer	EPSRC	Class2a	Dr Huasheng Wang	300.0	38.7	261.3
e258	Morphology and electronic props of semiconducting polymers	EPSRC	Class1b	Prof Alessandro Troisi	5,650.0	5,336.0	314.0
e260	Microscopic gas diffusion-reaction model	EPSRC	Class1a	Dr Jochen Blumberger	4,940.0	2,911.5	2,028.5
e261	Expressive and scalable finite element simulation	EPSRC	Class2b	Dr Garth Wells	800.0	45.6	754.4
e262	MC simulations of semiconductor nanostructures	EPSRC	Class2a	Prof Ian Galbraith	300.0	3.2	296.8
e263	Modelling the Elastic and Moisture Barrier Properties of Skin	EPSRC	Class1b	Dr Rebecca Notman	40,100.0	21,759.4	18,340.6
e264	Metabolic efficiency in neurons with extended morphology	EPSRC	Class2a	Dr Biswa Sengupta	300.0	213.8	86.2
e265	HPC for the Discrete Element Method User Community	EPSRC	Class2b	Dr Catherine O'Sullivan	800.0	0.0	800.0
e266	Thermal and Reactive Flow Simulation on High-End Computers	EPSRC	Class1a	Prof Kai Luo	226,800.0	2,078.6	224,721.4
e267	Simulating free-surface flow and fluid-structure interaction	EPSRC	Class2a	Dr Ido Akkerman	300.0	0.1	299.9
e268	Modelling of marine renewable energy farms	EPSRC	Class1a	Dr Bjoern Elsaesser	10,000.0	0.0	10,000.0
e269	Atomic data for fusion diagnostics	EPSRC	Class1b	Dr Catherine C A E Ramsbottom	4,870.0	0.0	4,870.0
e270	Turbulent mass transfer at high Schmidt number	EPSRC	Class1b	Dr Maarten van Reeuwijk	17,000.0	0.0	17,000.0
e271	Cloverleaf: preparing hydrodynamics codes for exascale	EPSRC	Class1b	Dr Stephen Jarvis	20,430.0	36.7	20,393.3
e272	TOUCAN: TOwards an Understanding of CAtalysis on Nanoalloys	EPSRC	Class1a	Prof Roy L. Johnston	187,000.0	1,813.4	185,186.6

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e273	Investigation of optimal control of laminar/turbulence flow	EPSRC	Class2a	Dr Xuerui Mao	300.0	189.5	110.5
e274	Characterization of the dynamics of alpha-synuclein	EPSRC	Class2a	Prof Michele Vendruscolo	400.0	320.2	79.8
e275	Harmonic Generation in Time Dependent R-matrix Theory	EPSRC	Class2a	Dr Hugo van der Hart	300.0	131.8	168.2
e277	Cellular automata simulation of microstructure evolution	EPSRC	Class2a	Dr Anton Shterenlikht	300.0	17.3	282.7
e278	Ab-initio investigation of Beryllium intermetallic compounds	EPSRC	Class2a	Mr Patrick A Burr	300.0	276.4	23.6
e279	Characterisation of the triplet excited state potential	EPSRC	Class2a	Dr Paul Elliott	300.0	17.5	282.5
e280	UK High-End Computing Consortium for Biomolecular Simulation	EPSRC	Class1a	Prof. Adrian Mulholland	1,075,000.0	0.0	1,075,000.0
e281	Plasma Physics Consortium	EPSRC	Class1a	Dr Tony Arber	500,000.0	0.0	500,000.0
e282	SI2-CHE: Chemical Software	EPSRC	Class1a	Dr Lorna Smith	20,472.0	0.0	20,472.0
e283	UK Consortium on Mesoscopic Engineering Sciences	EPSRC	Class1a	Prof Kai Luo	403,000.0	0.0	403,000.0
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71,990.7	22,478.4	49,419.5
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Adrian Wander	113,303.7	54,907.8	58,395.9
STFC Projects							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	13,002.7	9,795.7	3,207.0
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	355,961.9	229,065.6	126,896.3
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Grenville GMS Lister	884,900.8	595,418.0	289,482.8

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	765,654.7	529,240.1	236,414.6
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	254,510.5	138,937.5	115,573.0
n99	NERC Training	NERC	Class1a	Dr Grenville GMS Lister	2.0	0.0	2.0
BBSRC Projects							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000.0	1,394.4	605.6
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000.0	640.8	9,359.2
b12	Flu Analysis on HECToR	BBSRC	Class1a	Mr Adrian Jackson	50.0	0.0	50.0
b13	Linear Scaling DFT for Biochemistry Applications	BBSRC	Class1a	Dr David Bowler	5,587.2	105.6	5,481.6
b14	Understanding supercoiling-dependent DNA recognition	BBSRC	Class1a	Prof Anthony Maxwell	42,600.0	27,455.9	15,144.1
b15	Simulating bird and dinosaur footprints	BBSRC	Class2a	Dr Peter L Falkingham	300.0	31.2	268.8
Director's Time							
b10	SPRINTing with HECToR [dCSE]	DirectorsTime	Class2b	Mr Terry Sloan	4,595.1	521.3	4,073.8
d04	MSc in HPC	DirectorsTime	Service	Dr David Henty	613.5	478.1	135.4
d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	10,000.0	5,530.8	4,469.2
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	252.0	109.2	142.8
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1,000.0	18.6	981.4
d24	SBSI	DirectorsTime	Service	Dr Stephen Gilmore	2,000.0	958.1	1,041.9

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
d25	Code Scaling	DirectorsTime	Service	Dr Ken Rice	51,500.0	18,712.8	32,787.2
d26	Guest Training Accounts	DirectorsTime	Service	Miss Elizabeth Sim	1,250.0	903.0	347.0
d29	Nu-FuSe	DirectorsTime	Service	Mr Adrian Jackson	1,500.0	813.4	686.6
d32	APOS-EU	DirectorsTime	Service	Dr Michele Weiland	1,500.0	999.5	500.5
d34	Msc 2011-2012	DirectorsTime	Service	Dr David Henty	1,000.0	189.6	810.4
d35	PhD	DirectorsTime	Service	Dr Mark Bull	10.0	0.0	10.0
d36	Genome	DirectorsTime	Service	Dr Alan Gray	3,460.0	0.0	3,460.0
d37	CRESTA	DirectorsTime	Service	Dr Lorna Smith	21,000.0	11,862.2	9,137.8
d39	NCSA access	DirectorsTime	Service	Mr Mark A Straka	1,000.0	986.1	13.9
d40	Computational Chemistry at St Andrews	DirectorsTime	Service	Dr Herbert Fruchtl	2,000.0	411.8	1,588.2
d41	NPL Project	DirectorsTime	Service	Dr Ulrich Zachariae	90,000.0	48,498.7	41,501.3
d42	Oxford Nanopore Technologies	DirectorsTime	Service	Dr Jayne Wallace	1,170.2	734.2	436.0
d43	ECDF	DirectorsTime	Class2b	Mr Tony Weir	25,000.0	6,979.0	18,021.0
d44	Crucible	DirectorsTime	Service	Mr Iain A Bethune	1,000.0	0.0	1,000.0
d45	MSc in HPC 2012-2013	DirectorsTime	Service	Dr David Henty	1,000.0	96.3	903.7
d46	Silicate melts with CP2K	DirectorsTime	Service	Mr Iain A Bethune	500.0	0.2	499.8
d47	PGS Project	DirectorsTime	Service	Dr Kevin Stratford	100.0	0.1	99.9

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
d49	Leiden	DirectorsTime	Service	Dr. Simon Portegies Zwart	200.0	0.7	199.3
External Projects							
e168	TEXT	External	Service	Dr Mark Bull	1,500.0	79.5	1,420.5
PRACE Projects							
pr1u0702	HYDROGEN-ILs	PRACE	Class1a	Dr Chris A Johnson	770332.7	8618.0	761714.7
pr1u0705	TanGrin	PRACE	Class1a	Dr Chris A Johnson	14084.0	14042.1	41.9
pr1u0804	FULLDRUG	PRACE	Class1a	Dr Chris A Johnson	15064.0	15062.6	1.4
pr1u0806	NELC	PRACE	Class1a	Dr Chris A Johnson	11408.0	4038.9	7369.1
pr1u0807	PARAMETER	PRACE	Class1a	Dr Chris A Johnson	6720.0	5738.1	981.9
pr1u0809	VIPforVPH	PRACE	Class1a	Dr Chris A Johnson	5346.0	1161.9	4184.1
pr1u0810	DrugEffluxMechanism	PRACE	Class1a	Dr Chris A Johnson	4964.8	0.0	4964.8
pr1u0902	ESM4OED	PRACE	Class1a	Dr Chris A Johnson	10272.0	4002.1	6269.9
pr1u0903	ICREIMUTANTS	PRACE	Class1a	Dr Chris A Johnson	3766.0	13.0	3753.0
pr1u0904	MoMoGal	PRACE	Class1a	Dr Chris A Johnson	23976.0	4899.2	19076.8
pr1u0905	MPI-FETI	PRACE	Class1a	Dr Chris A Johnson	9096.0	204.9	8891.1
pr1u0906	FORSQUALL	PRACE	Class1a	Dr Chris A Johnson	3156.0	1.4	3154.6
pr1u0907	GPCR4D	PRACE	Class1a	Dr Chris A Johnson	2259.8	958.9	1300.9

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pr1u9999	PRACE Training	PRACE	Class1a	Dr David Henty	0.0	0.0	0.0