



HECToR Quarterly Report

Apr - Jun 2012

1 Introduction

This report covers the period from 1 April 2012 at 0800 to 1 July 2012 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/2Q12.php>

2 Executive Summary

- XE6 utilisation in 2Q12 was 68%, which was the same as 1Q12. The double bank holiday period in early June has had a clear impact on utilisation, with less usage in June. Further details are available in Section 3.2 of the report.
- There were 3 service failures in 2Q12 as opposed to 5 in 1Q12. There was one maintenance overrun, one job scheduling issue, and one filesystem issue. The overall MTBF improved on 1Q12 from 439 hours to 732 hours.
- The volume of single node failures remained low. Node failures may impact single user jobs, but we no longer experience the system-wide issues we used to see as a result.
- HECToR was integrated into the Research Data facility (RDF) in May. The RDF comprises of 7.8PB of disk storage, with 19.5PB of backup tape. Users from 10 EPSRC and 4 NERC consortia now have access to the disk. Work will continue in 3Q12 to enhance the mechanisms in place for transferring data to/from the RDF to HECToR, the NERC LMS and external sites.
- New queues supporting 24 hour jobs were introduced on 4th July. These will be available for an initial 6 month trial period. Previously the longest job that could be supported outside a special reservation was 12 hours. To date in July, these longer jobs have accounted for around 12% of the overall utilisation.
- An additional 6 PRACE funded projects came online on HECToR in late June, bringing the total to 9 active projects. We therefore expect the PRACE utilisation on HECToR to rise closer to the PRACE 5% allocation in the coming quarter.

3 Quantitative Metrics

3.1 Reliability

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

	Apr	May	Jun
Incidents	7	11	10
Failures	0	1	2

3.1.1 Performance Statistics

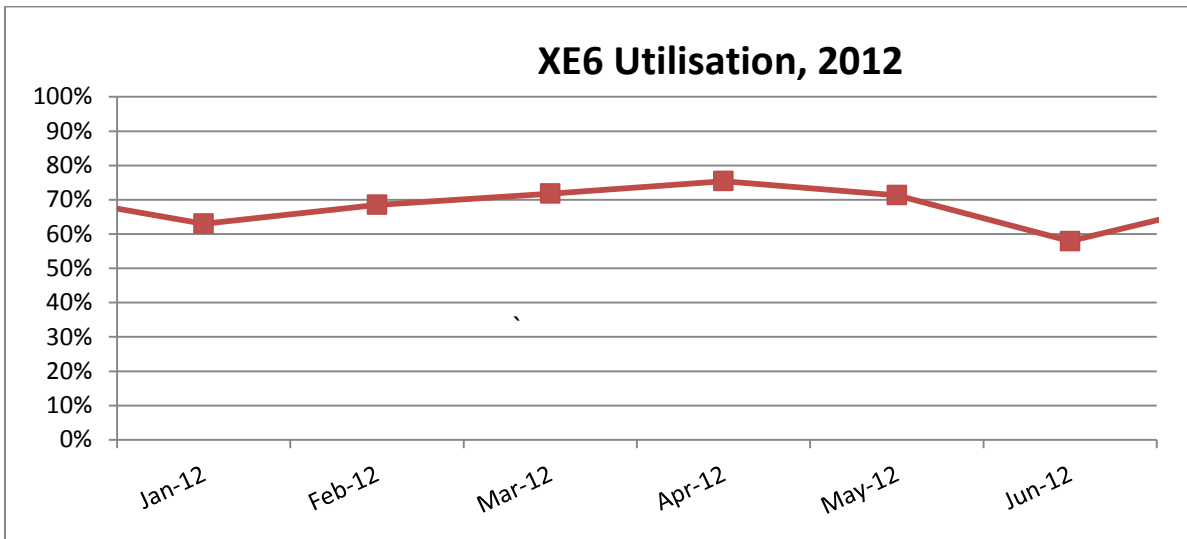
$MTBF = (732)/(\text{number of failures in a month})$

$\text{Quarterly MTBF} = (3 \times 732)/(\text{number of failures in a quarter})$

Attribution	Metric	Apr	May	Jun	Quarterly
Technology	Failures	0	1	2	3
	MTBF	∞	732	366	732
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	0	1	2	3
	MTBF	∞	732	366	732

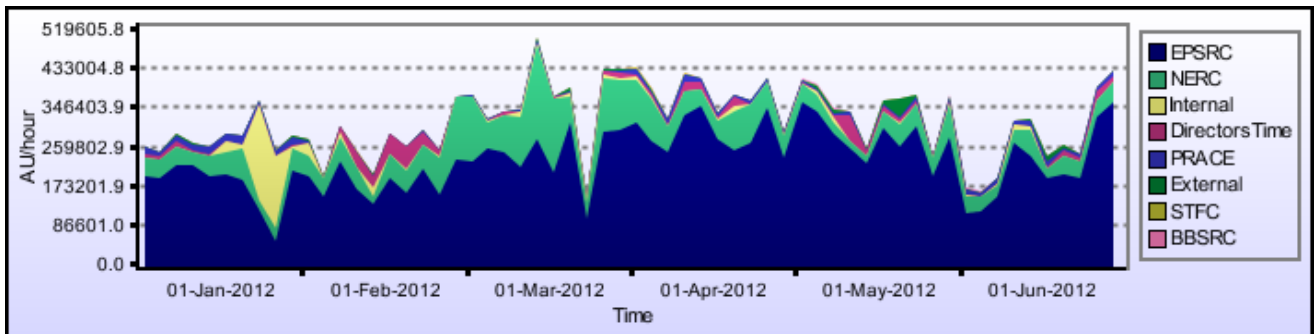
3.2 HECToR Utilisation

3.2.1 XE6 Utilisation



The XE6 utilisation quarterly average in 2Q12 was 68.2%, compared to 67.8% in 1Q12.

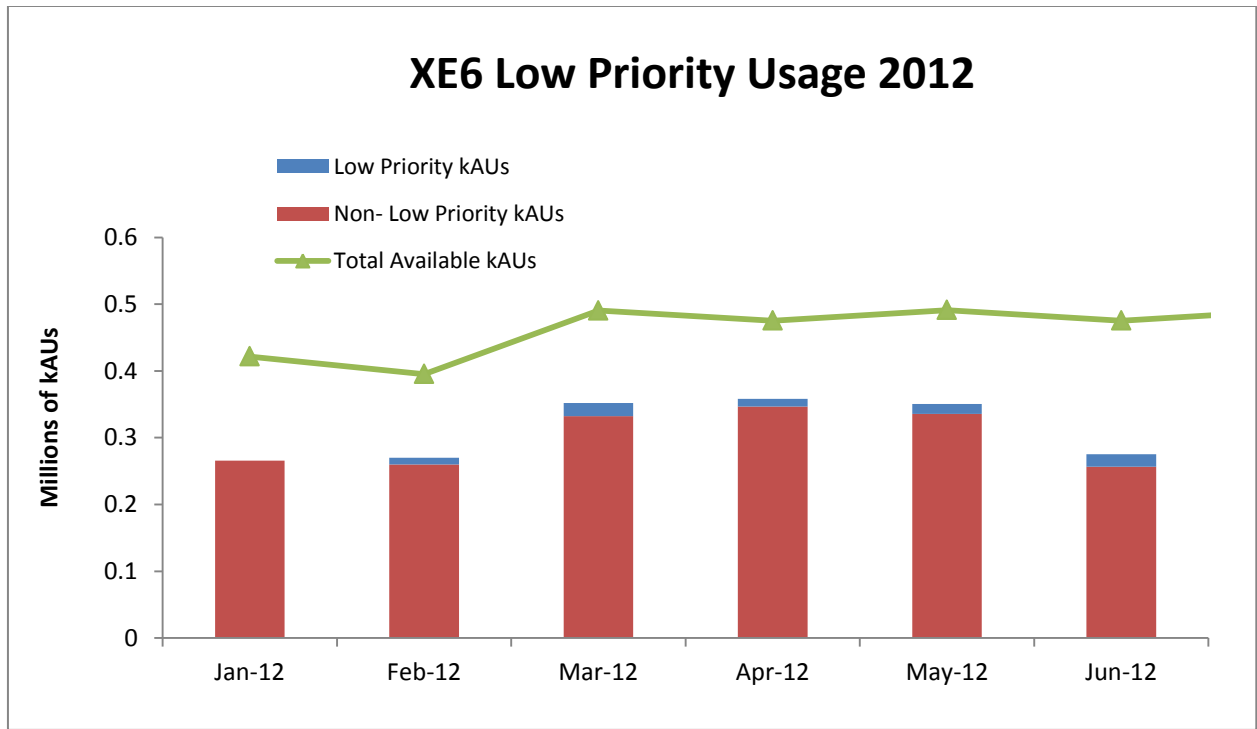
Capability Usage



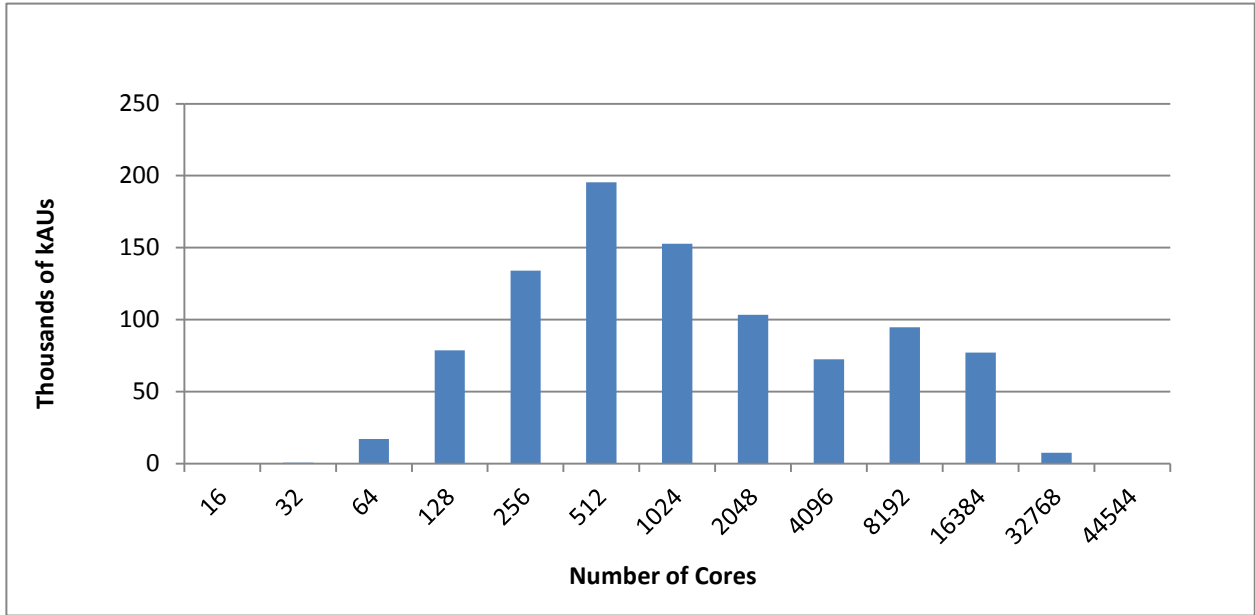
Raw AUs use by Funding Body of jobs using more than 511 CPUs

Low Priority Access

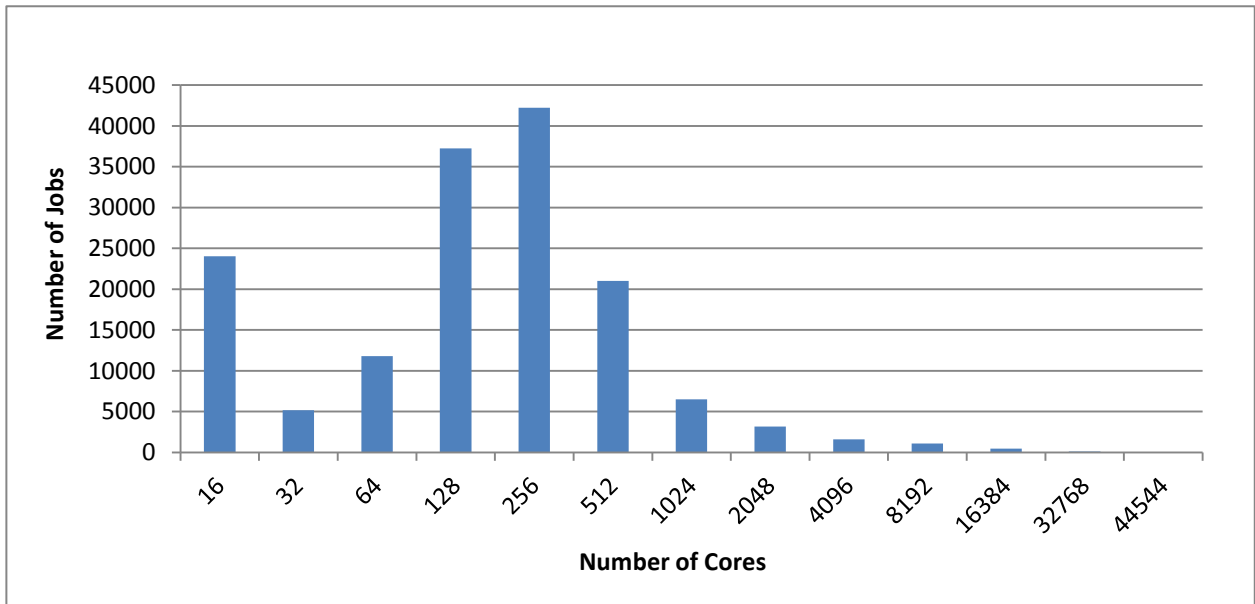
In 2Q12, low priority access accounted for 4.8% of the overall utilisation.



3.2.2 Utilisation by Core Count



3.2.3 Number of Jobs by Core Count



3.2.4 Utilisation by Consortium

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
y01	0.0	0.0	1	0.00%
y02	3.0	5.7	16	0.00%
y03	575.1	564.2	1321	0.04%
y07	2.5	4.6	248	0.00%
z01	1210.0	2260.8	372	0.16%
z02	77.3	144.4	16	0.01%
z03	2358.0	4407.8	986	0.31%
Internal Total	4225.9	7387.4	2960	0.51%
c01	5889.2	10979.6	2057	0.76%
e01	13913.5	29074.0	3528	2.02%
e05	167176.9	312305.8	35205	21.66%
e10	4678.7	8745.7	1528	0.61%
e68	96.4	180.3	10	0.01%
e71	1035.0	1934.7	340	0.13%
e76	3456.5	6460.6	285	0.45%
e82	0.8	1.5	2	0.00%
e89	36571.6	81266.6	11336	5.64%
e104	827.1	1546.0	602	0.11%
e106	0.3	0.6	1	0.00%
e107	0.2	1090.8	190	0.08%
e108	7415.1	13859.5	733	0.96%
e110	9722.1	18399.4	1479	1.28%
e122	12039.9	22633.9	1022	1.57%
e124	4300.2	18628.9	936	1.29%
e125	10572.1	19760.5	445	1.37%
e126	2207.5	4126.0	45	0.29%
e127	388.3	725.9	13	0.05%
e128	166.0	310.3	73	0.02%
e129	74.4	139.0	62	0.01%
e130	414.2	774.1	116	0.05%
e141	479.3	895.8	462	0.06%
e145	16.5	30.9	11	0.00%
e149	563.4	1053.1	129	0.07%
e156	45.0	84.1	22	0.01%
e158	0.0	0.0	3	0.00%
e159	0.1	0.1	85	0.00%
e160	7794.3	14647.5	385	1.02%
e163	99.6	186.2	126	0.01%
e173	476.0	889.7	480	0.06%
e174	492.4	920.4	92	0.06%
e175	0.0	313.4	1	0.02%
e177	1980.9	3702.5	976	0.26%
e179	170.7	319.1	79	0.02%
e184	610.8	1141.6	196	0.08%
e186	15997.8	29901.7	1039	2.07%
e187	210.8	394.2	470	0.03%
e193	7985.8	14932.6	728	1.04%
e203	551.4	1030.8	241	0.07%
e204	10.4	19.5	2	0.00%
e207	5566.5	10404.4	5	0.72%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
e210	3.2	5.9	19	0.00%
e213	0.3	0.6	32	0.00%
e215	440.0	822.4	34	0.06%
e220	15305.3	45230.0	1016	3.14%
e224	42.6	79.6	51	0.01%
e225	167.0	312.2	44	0.02%
e228	192.2	359.2	167	0.02%
e229	6316.9	11807.0	1090	0.82%
e230	11.3	21.1	2	0.00%
e231	83.1	155.3	101	0.01%
e232	208.1	389.0	139	0.03%
e233	628.9	1175.5	217	0.08%
e234	904.1	1689.8	163	0.12%
e235	176.7	330.4	281	0.02%
e236	0.0	0.0	23	0.00%
e237	353.0	659.7	416	0.05%
e238	342.0	639.3	68	0.04%
e240	118.9	222.3	218	0.02%
e241	1.2	2.2	26	0.00%
e244	1.4	2.7	377	0.00%
e245	58.3	108.9	130	0.01%
e247	220.9	412.8	76	0.03%
e249	553.8	1035.2	53	0.07%
e250	165.3	309.0	13	0.02%
e251	3072.3	5742.4	145	0.40%
e252	3632.1	6788.8	365	0.47%
e253	8.4	15.7	36	0.00%
j01	945.5	1767.3	484	0.12%
EPSRC Total	357950.8	713895.9	71326	49.51%
n01	19165.1	35821.8	4280	2.48%
n02	36322.6	67903.8	47412	4.71%
n03	40599.8	75886.9	5505	5.26%
n04	10030.5	18752.7	6399	1.30%
NERC Total	106117.9	198365.2	63596	13.76%
b09	0.5	0.9	6	0.00%
b10	0.0	0.0	11	0.00%
b14	1528.8	2857.6	386	0.20%
b100	3.5	6.5	134	0.00%
BBSRC Total	1532.8	2864.9	537	0.20%
p01	739.0	1381.2	44	0.10%
STFC Total	739.0	1381.2	44	0.10%
e168	3.4	6.3	90	0.00%
x01	7945.2	14851.1	5243	1.03%
x08	0.0	0.0	2	0.00%
x10	19.4	36.3	80	0.00%
External Total	7967.9	14893.7	5415	1.03%
d04	0.0	0.0	1	0.00%
d11	2302.9	4304.3	140	0.30%
d15	1.0	1.9	35	0.00%
d23	0.4	0.7	38	0.00%
d25	1607.3	3004.2	725	0.21%
d26	325.6	406.0	1068	0.03%
d27	5.0	9.3	104	0.00%
d29	31.1	58.2	117	0.00%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
d32	60.8	113.8	386	0.01%
d34	32.8	57.3	370	0.00%
d37	1832.8	3425.7	1325	0.24%
d38	231.6	433.0	286	0.03%
d39	151.2	285.5	366	0.02%
d40	116.7	218.2	59	0.02%
d41	5619.4	10503.3	2453	0.73%
d42	734.1	1372.1	83	0.10%
gd11	0.0	0.0	2	0.00%
x07	6.7	12.6	34	0.00%
DirectorsTime Total	13059.5	24206.1	7592	1.68%
pr1u0704	3413.1	6380.2	175	0.44%
pr1u0705	5639.4	10540.6	344	0.73%
pr1u0804	2162.6	4042.2	2617	0.28%
pr1u0809	0.1	0.1	6	0.00%
PRACE Total	11215.2	20963.1	3142	1.45%
Total	502809.0	983957.5	154612	68.24%

3.3 Helpdesk

A total of 1112 queries with a specified service metric and *577 queries with no metric were completed in this period.

*Setup tickets for the RDF have no metric associated as the RDF support is on a reasonable endeavours basis only. These tickets are not included in the summary below.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	942	947	99.5%	97.0%
Admin queries finished in 1 day	876	881	99.4%	97.0%
Queries assigned in 30 min	1100	1105	99.5%	97.0%
Technical assessments in 10 days	25	25	100.0%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	586	52.7%
Admin	295	26.5%
In-depth	140	12.6%
Technical	66	5.9%
Technical assessment	25	2.2%

Queries by Category

Query Category	Queries	Percentage
New User	141	12.7%
Set user quotas	126	11.3%
New Password	116	10.4%
Set group quotas	94	8.5%
3rd Party Software	84	7.6%
Disk, tapes, resources	63	5.7%
Batch system and queues	63	5.7%
Access to HECToR	60	5.4%
User behaviour	47	4.2%
None	43	3.9%
Compilers and system software	42	3.8%
User programs	33	3.0%
Login, passwords and ssh	28	2.5%
New Group	25	2.2%
Join Project	22	2.0%
Make Reservation	21	1.9%
Add to group	21	1.9%
Courses	15	1.3%
Create certificate	14	1.3%
Other	9	0.8%
Node Failure	8	0.7%
Archive	8	0.7%
Static website	5	0.4%
SAFE	5	0.4%
Performance and scaling	5	0.4%
Grid	5	0.4%
Remove account	4	0.4%
gpu	2	0.2%
Update account	2	0.2%
Network	1	0.1%

Queries by Handler Category

Handlers	Admin	In-depth	Technical	Automatic	TA	Total	%age
USL	244	30	50	0	0	324	29.1%
CSE	2	80	0	0	25	107	9.6%
OSG	47	6	4	586	0	643	57.8%
Cray	2	24	12	0	0	38	3.4%

3.3.1 Quality Tokens

A number of positive quality tokens were received in 2Q12. There were no negative tokens.

Project	Positive Tokens	Negative Tokens
d37	3	0
x10	5	0
Total	8	0

3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Apr-12	May-12	Jun-12	2Q12
Technology Reliability (%)	85.00%	98.50%	100.0%	96.8%	99.5%	98.7%
Technology MTBF (hours)	100	126.4	∞	732	366	732
Technology Throughput, hours/year	7000	8367	8681	8365	8603	8550
Capability jobs completion rate	70%	90%	100.0%	100.0%	100%	100%
Non in-depth queries resolved within 1 day (%)	85%	97%	100.0%	99.1%	99.2%	99.4%
Number of SP FTEs	7.3	8.0	8.4	8.8	8.2	8.5
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

$$\text{SP Serviceability\%} = 100 * (\text{WCT} - \text{SDT} - \text{UDT}(\text{SP})) / (\text{WCT} - \text{SDT})$$

$$\text{Technology Reliability \%} = 100 * (1 - (\text{UDT}(\text{Technology}) / (\text{WCT} - \text{SDT})))$$

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 Richard Blake	50,803.70	46,318.90	4,484.10
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969.90	118,378.00	365,454.70
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124.00	634,273.00	504,175.50
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257,748.20	15,231.30	242,516.90
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000.00	49,887.50	112.5
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403.50	53,807.80	76,584.00
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521.80	40,208.70	2,313.10
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105.40	867.6	237.7
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600.00	3,203.10	6,396.90
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088.60	6,286.80	1,801.80
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	400,100.00	342,671.00	57,429.00
e92	Dynamo Action In Compressible Convection	EPSRC	Class1a	Mr Paul Bushby	4,075.00	4,074.40	0.6
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400.00	8,465.10	21,934.90
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1a	Dr Andreas M Kempf	1,300.00	297.3	1,002.70

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1a	Prof Kai Luo	3,650.00	93.2	3,556.80
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000.00	720.9	5,279.10
e108	Jet Flap Noise	EPSRC	Class1a	Dr Sergey Karabasov	49,684.50	26,401.40	23,283.00
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	140,110.30	75,814.30	64,234.00
e121	[dCSE] Improving Performance using Wannier functions	EPSRC	Class1a	Prof Maria Merlyne DeSouza	2,680.30	2,299.60	380.7
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	150,000.00	69,684.30	80,315.70
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887.90	17,263.10	5,616.80
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168,324.80	32,670.80	135,544.10
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584.00	16,843.50	8,740.50
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000.00	1,971.30	5,028.70
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7,092.10	4,123.80	2,968.30
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500.00	1,573.70	5,926.30
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500.00	2,777.80	7,722.20
e141	A numerical study of turbulent manoeuvring-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350.00	4,609.10	11,740.90
e144	Numerical Simulation of Rotating Stall and Surge	EPSRC	Class1a	Dr Mehdi Vahdati	1,266.00	0.3	1,265.70
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191.90	402.2	787.2
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082.50	48,496.60	19,585.90

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000.00	161.7	9,838.30
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600.00	163.1	1,436.90
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	500	423.5	76.5
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3,816.00	29.7	3,786.30
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208.10	8,953.20	11,254.90
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69,895.50	0	69,895.50
e163	Numerical Simulation of Spontaneous Ignition	EPSRC	Class1b	Prof Jennifer Wen	4,142.30	612.8	3,529.50
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4,872.00	0	4,872.00
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800.00	796.7	4,003.30
e174	3D instabilities in two-layer flows	EPSRC	Class1b	Dr Prashant Valluri	11,495.40	1,516.20	9,979.20
e175	Fine-Scale Turbulence	EPSRC	Class1a	Dr Richard D Sandberg	50,000.00	1,165.90	48,678.50
e177	Amorphous structures of mirror coatings	EPSRC	Class1b	Dr Ian Maclaren	5,700.80	3,049.90	2,650.90
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000.00	2,250.90	84,749.10
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8,150.20	0	8,150.20
e183	Analysis of Processes in Hydrocarbon Fuel Droplets	EPSRC	Class1a	Prof Sergei Sazhin	8,640.00	0	8,640.00
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130,500.00	1,343.20	129,156.80
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000.00	6,142.70	333,857.30

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70,000.00	46,105.90	23,894.10
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030.20	599.6	5,430.50
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40,500.00	4,413.10	36,086.90
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38,345.00	0	38,345.00
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim Biktashev	4,499.60	1,360.60	3,139.00
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5,000.00	118.1	4,881.90
e206	FLAME Agent-Based Simulation Framework	EPSRC	Class1a	Prof Christopher Greenough	410	0	410
e207	Developing DL_POLY Molecular Dynamics Simulation code	EPSRC	Class1a	Dr Kostya Trachenko	25,857.60	8,720.80	17,136.90
e211	Dendrite simulation	EPSRC	Class1a	Dr Jiawei Mi	300	1.1	298.9
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	0.3	399.7
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26,121.60	17,391.80	8,729.80
e223	Numerical modelling of aorta dissection	EPSRC	Class2a	Prof. Xiaoyu Luo	300	0	300
e224	Electronic properties of inorganic-organic hybrid materials	EPSRC	Class2a	Prof Anthony K Cheetham	400	422.6	-22.6
e225	New Ru and Ir Chromophores for Solar Cell Devices	EPSRC	Class2a	Dr Paul Elliott	300	304.9	-4.9
e226	Novel Vibrational Spectroscopic Techniques	EPSRC	Class1a	Dr Andrew D Burnett	1,032.30	0	1,032.30
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50	46.4	3.6
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	20,218.30	345.9	19,872.40

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e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50,000.00	7,867.70	42,132.30
e230	Adsorption and Diffusion in Metal-Organic Frameworks	EPSRC	Class2a	Dr Ahmet Ozgur Yazaydin	918.9	517.4	401.5
e231	Rapid Alloy Solidification	EPSRC	Class1b	Prof Peter Jimack	5,130.00	285.8	4,844.20
e232	Flow field analysis around flap type wave energy devices	EPSRC	Class2a	Dr Matthew Folley	289.9	290.7	-0.9
e235	Modelling offshore wind	EPSRC	Class2a	Prof Simon Watson	400	217.1	182.9
e236	Simulations of Optical Communications Systems	EPSRC	Class2a	Dr Marc Eberhard	400	587.1	-187.1
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400	399	1
e239	Optimum Collection and Conversion of Light into Energy	EPSRC	Class2a	Dr Robert Paton	400	0	400
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	160.2	639.8
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	1.4	498.6
e242	Study of the Green Fluorescent Protein Fluorophore	EPSRC	Class2a	Dr Garth Jones	400	0	400
e243	Tailored Structures for Orthopaedic Implantations	EPSRC	Class2a	Dr Carmen Torres-Sanchez	400	0	400
e244	VOX-FE: Large Scale FE Bone Modelling on HECToR	EPSRC	Class2b	Prof Michael Fagan	800	1.7	798.3
e245	Parallelisation of a harmonic balance NS solver	EPSRC	Class2b	Dr Sergio Campobasso	800	104.4	695.6
e246	Numerical simulation of capillary blood flow	EPSRC	Class2a	Dr Ellak Somfai	400	0	400
e247	Tool development for multiscale protein folding simulations	EPSRC	Class2a	Dr Robert Best	400	220.9	179.1
e248	Testing of a Distributed Coordinate Descent Method	EPSRC	Class2a	Dr Peter Richtarik	400	0	400

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e249	Feedback flow control for reducing the aerodynamic drag	EPSRC	Class1b	Dr Aimee Morgans	9,860.00	858.2	9,001.80
e250	Thermal Mixing around In-line Tube Banks	EPSRC	Class1b	Prof Hector Iacovides	2,002.00	208.3	1,793.70
e251	Asynchronous Genetic Algorithms in HPC Gait Simulation	EPSRC	Class1b	Dr Bill Sellers	13,200.00	3,844.10	9,355.90
e252	LES of flows around wind turbine blades	EPSRC	Class1b	Dr Zheng-Tong Xie	7,740.00	3,798.60	3,941.40
e253	Turbulent premixed and stratified combustion	EPSRC	Class1b	Prof Stewart Cant	14,221.00	90	14,131.00
e254	Ceramic Composites for Fusion Power	EPSRC	Class1b	Prof Sergei Dudarev	8,371.00	0	8,371.00
e255	Turbulent Drag Reduction	EPSRC	Class2a	Dr Pierre Ricco	400	0	400
e256	Hybrid simulation on heat transfer	EPSRC	Class2a	Dr Huasheng Wang	300	0	300
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71,990.70	22,052.20	49,845.60
STFC Projects							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	10,002.70	1,845.00	8,157.70
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	220,690.90	166,120.60	54,570.30
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Grenville Lister	676,027.50	457,611.10	218,416.40
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	538,860.70	412,346.10	126,514.60
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	152,305.70	100,967.40	51,338.30
n99	NERC Training	NERC	Class1a	Dr Grenville Lister	2	0	2

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BBSRC Projects							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000.00	1,394.40	605.6
b10	SPRINTing with HECToR [dCSE]	BBSRC	Class2b	Mr Terry Sloan	1,595.10	519.1	1,076.10
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000.00	636	9,364.00
b12	Flu Analysis on HECToR	BBSRC	Class1a	Mr Adrian Jackson	50	0	50
b13	Linear Scaling DFT for Biochemistry Applications	BBSRC	Class1a	Dr David Bowler	5,587.20	105.6	5,481.60
b14	Understanding supercoiling-dependent DNA recognition	BBSRC	Class1a	Prof Anthony Maxwell	42,600.00	1,698.70	40,901.30
Director's Time							
d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	10,000.00	2,438.30	7,561.70
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	102	3.9	98.2
d19	OpenFOAM Demo	DirectorsTime	Service	Dr Alan Gray	1,950.00	1,894.80	55.2
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1,000.00	18.6	981.4
d23	TEXT FP7	DirectorsTime	Service	Dr Mark Bull	1,500.00	35.2	1,464.80
d24	SBSI	DirectorsTime	Service	Dr Stephen Gilmore	2,000.00	958.1	1,041.90
d25	Code Scaling	DirectorsTime	Service	Dr Ken Rice	51,500.00	6,803.70	44,696.30
d26	Guest Training Accounts	DirectorsTime	Service	Miss Elizabeth Sim	50	44.2	5.8
d27	Rolls	DirectorsTime	Service	Mr Paul Graham	50	40.7	9.3

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d28	Simulations of antimicrobial peptides	DirectorsTime	Service	Dr Andrew R Turner	7,641.70	7,641.70	0
d29	Nu-FuSe	DirectorsTime	Service	Mr Adrian Jackson	500	0.9	499.1
d30	PARTRAC	DirectorsTime	Service	Dr Mark Sawyer	200	124	76
d31	Semileptonic Decay	DirectorsTime	Service	Prof Richard Kenway	1,000.00	0	1,000.00
d32	APOS-EU	DirectorsTime	Service	Dr Michele Weiland	1,000.00	143.3	856.7
d33	Mark Westwood's Project	DirectorsTime	Service	Mr Mark Westwood	100	8.9	91.1
d34	Msc 2011-2012	DirectorsTime	Service	Dr David Henty	1,000.00	61.3	938.7
d35	PhD	DirectorsTime	Service	Dr Mark Bull	10	0	10
d36	Genome	DirectorsTime	Service	Dr Alan Gray	3,460.00	0	3,460.00
d37	CRESTA	DirectorsTime	Service	Dr Lorna Smith	11,000.00	1,117.20	9,882.80
d38	Windfarm Simulation	DirectorsTime	Service	Mr Adrian Jackson	171	81.1	89.9
d39	NCSA access	DirectorsTime	Service	Mr Mark A Straka	1,000.00	799.9	200.1
d40	Computational Chemistry at St Andrews	DirectorsTime	Service	Dr Herbert Fruchtl	2,000.00	16.9	1,983.10
d41	NPL Project	DirectorsTime	Service	Dr Ulrich Zachariae	45,000.00	10,898.00	34,102.00
d42	Oxford Nanopore Technologies	DirectorsTime	Service	Dr Jayne Wallace	400	0.1	399.9
d43	IS Apps	DirectorsTime	Service	Mr Tony Weir	1,000.00	0	1,000.00
d44	Crucible	DirectorsTime	Service	Mr Iain A Bethune	1,000.00	0	1,000.00

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External Projects							
x01	HPC-Europa	External	Service	Dr Judy Hardy	38,762.40	29,909.30	8,853.10
x05	FIOS	External	Service	Mr Davy Virdee	1,130.10	1,076.60	53.5
x06	Rhymney	External	Service	Dr Mark Sawyer	4.5	0.1	4.4
x08	Marine Institute Ireland	External	Service	Dr Alan Berry	100	35.8	64.2
PRACE Projects							
pr1u0704	HIFLY	PRACE	Class1a	Dr Chris A Johnson	8,450.40	4,663.50	3,786.90
pr1u0705	TanGrin	PRACE	Class1a	Dr Chris A Johnson	14,084.00	7,519.00	6,565.00
pr1u0706	SIVE-2	PRACE	Class1a	Dr Chris A Johnson	14,000.00	5,213.60	8,786.40
pr1u0804	FULLDRUG	PRACE	Class1a	Dr Chris A Johnson	14,874.00	3,205.70	11,668.30
pr1u0805	NanoTherm	PRACE	Class1a	Dr Chris A Johnson	7,168.00	0	7,168.00
pr1u0806	NELC	PRACE	Class1a	Dr Chris A Johnson	11,408.00	0	11,408.00
pr1u0807	PARAMETER	PRACE	Class1a	Dr Chris A Johnson	6,720.00	0	6,720.00
pr1u0808	PIPETURB	PRACE	Class1a	Dr Chris A Johnson	12,600.00	0	12,600.00
pr1u0809	VIPforVPH	PRACE	Class1a	Dr Chris A Johnson	5,346.00	0.1	5,345.90