HECToR Quarterly Report

Oct - Dec 2011

1 Introduction

This report covers the period from 1 October 2011 at 0800 to 1 Jan 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/4Q11.php

2 Executive Summary

- 4Q11 was a busy period for the service with the upgrade to Phase 3. The upgrade was initially planned in a number of stages running from early November through to December. The system was downsized from 20 to 10 cabinets on 7th November as originally planned, but then remained at a reduced capacity until 7th December. During this period extensive testing was carried out on the new processors. The system returned as a 20 cabinet Interlagos solution on 7th December, and the final 10 cabinets were introduced on 18th January. A full review of the Phase 3 hardware changes will be included in the Annual Report.

- XE6 utilisation in 4Q11 was 73%, compared to 63% in 3Q11. Further details are available in Section 3.2 of the report. Charging was suspended on 7th November when the system was downsized in readiness for the Phase3 upgrade. This remained disabled for the remainder of the quarter. Details are available in Section 3.2 of this report.

- There were 4 service failures in 4Q11 as opposed to 1 in 3Q11. There was one maintenance overrun, one file system problem, and two plant-related issues. The overall MTBF was 549 hours which is ahead of target. A summary of all service failures over the year will be included in the Annual Report.

- The volume of single node failures remained constant from the previous quarter.

- The helpdesk statistics were again excellent. 15 positive and no negative quality tokens were received from users in 4Q11.

- The first batch of HECToR users as part of the PRACE initiative came online in November.

- The Invitation To Tender for the Tertiary Storage solution was published in December with to the expectation of having a solution in place in spring 2012.

3 Quantitative Metrics

3.1 Reliability

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

	Oct	Nov	Dec
Incidents	10	2	25
Failures	0	3	1

3.1.1 Performance Statistics

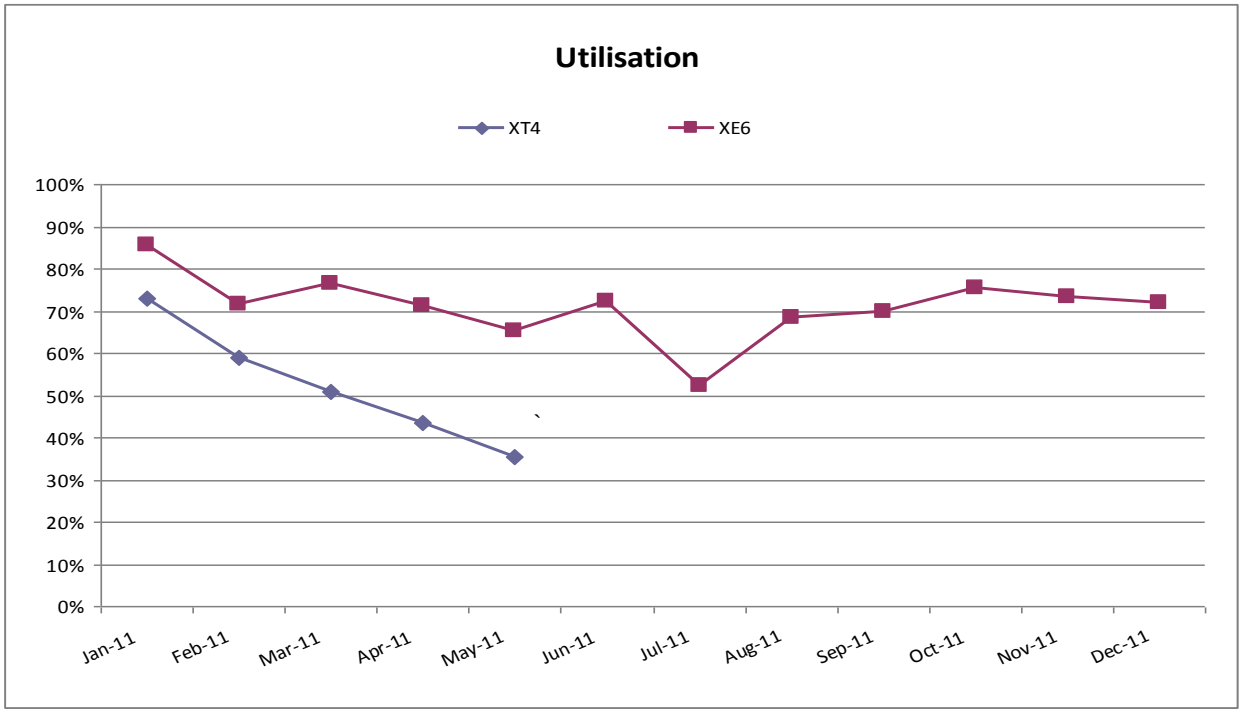
MTBF = (732)/(number of failures in a month)

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

Attribution	Metric	Oct	Nov	Dec	Quarterly
Technology	Failures	0	1	1	2
	MTBF	∞	732	732	1098
Service Provision	Failures	0	2	0	2
	MTBF	∞	366	∞	1098
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	0	3	1	4
	MTBF	∞	**244**	**732**	**549**

3.2 HECToR Utilisation

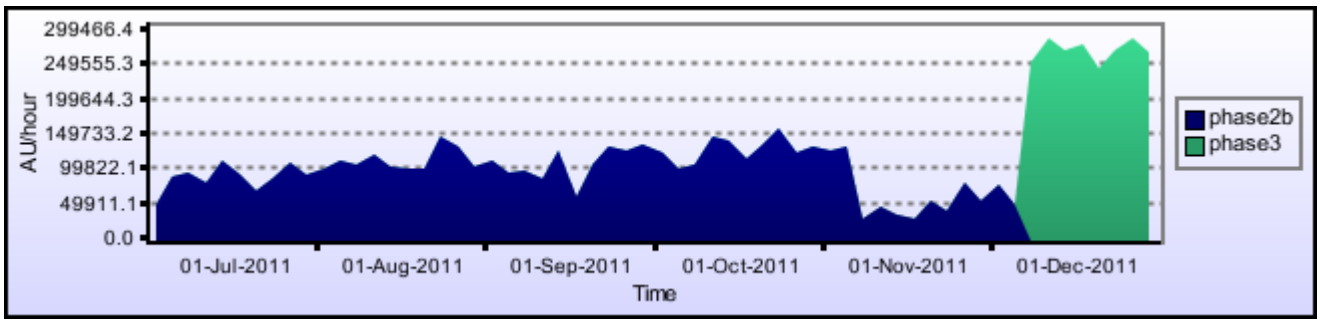
3.2.1 XE6 Utilisation



The XT4 utilisation quarterly average in 4Q11 was 73%, compared to 63% in 3Q11.

Capability Usage

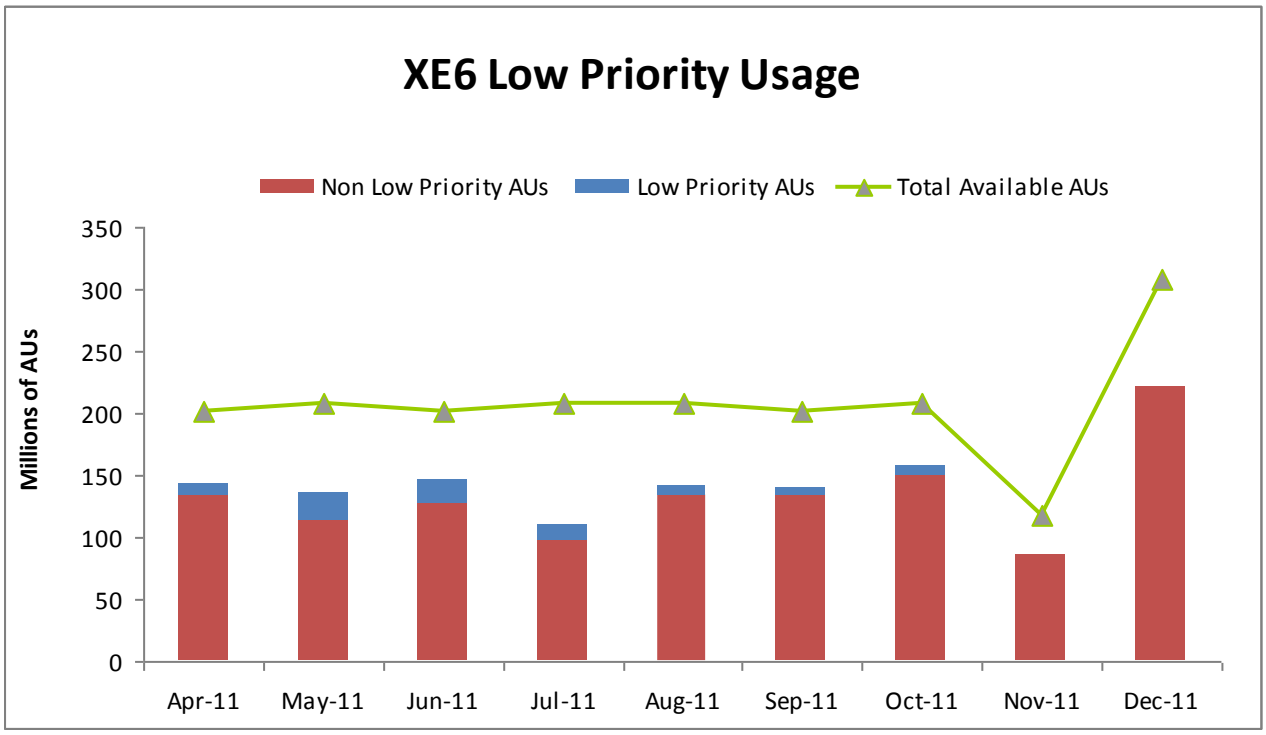
The arrival of Phase3 and the increased capacity on the service in December can clearly be seen below. The dip in November can be attributed to the period when HECToR was run at half capacity whilst testing on the new Phase3 architecture continued.



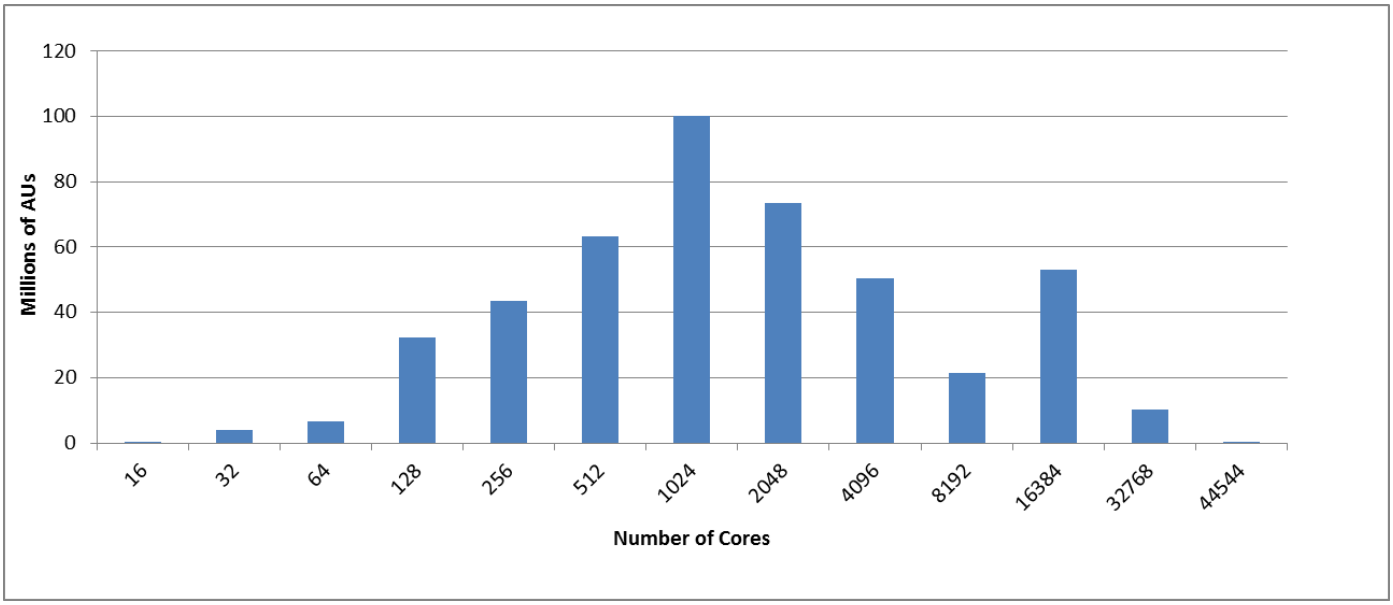
RawAUs use by Machine of jobs using more than 511 CPUs

Low Priority Access

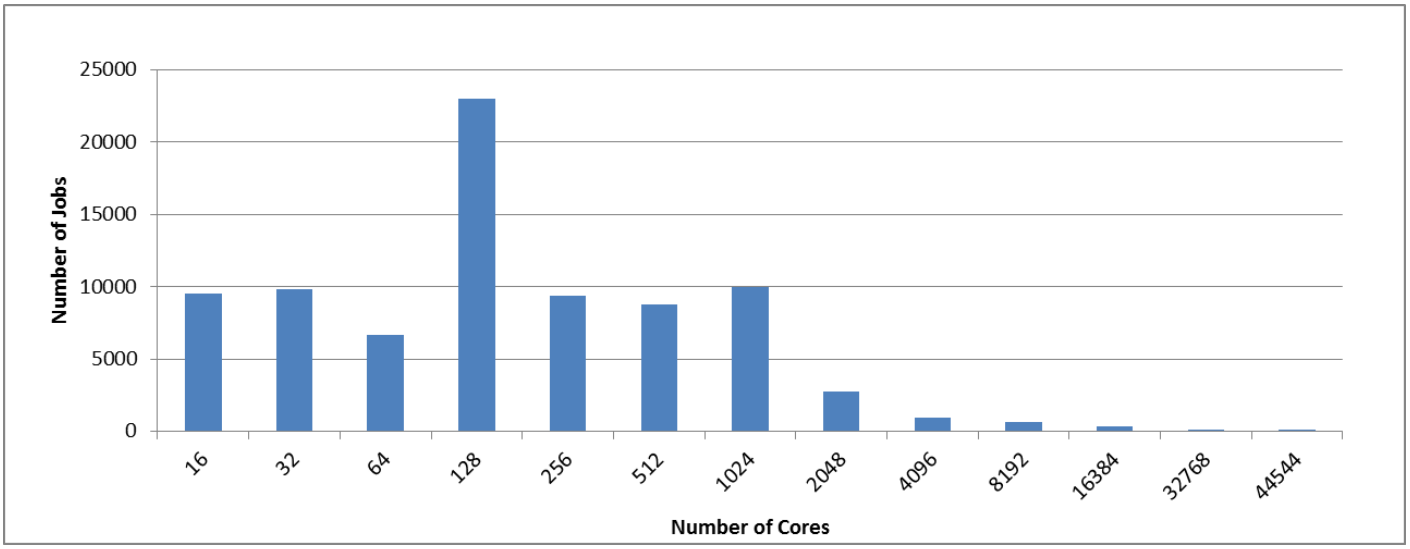
In 4Q11, low priority access accounted for 2.1% of the overall utilisation. This was disabled during November when the machine was operating at half capacity and during December when charging was disabled.



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	0.5	2	0.0%
y02	11.3	1263.5	146	0.2%
y03	412.7	371.3	469	0.1%
y05	0.0	0.0	4	0.0%
y07	0.0	0.8	151	0.0%
z01	36.9	299.2	559	0.1%
z03	1471.5	3271.2	1475	0.5%
Internal Total	1932.4	5206.5	2806	0.8%
c01	347.9	767.5	1181	0.1%
e01	8489.7	31752.9	1869	5.0%
e05	25931.0	91888.7	15284	14.5%
e10	25.0	50.9	48	0.0%
e68	14.5	30.6	21	0.0%
e71	424.7	2839.0	422	0.5%
e76	15.7	79.1	32	0.0%
e82	0.2	42.2	105	0.0%
e85	1439.8	8768.6	131	1.4%
e89	17070.4	49496.3	6986	7.8%
e92	35.1	43.8	7	0.0%
e104	121.5	288.1	223	0.1%
e107	0.1	8313.7	164	1.3%
e108	1305.1	1765.4	293	0.3%
e110	1133.9	10117.4	714	1.6%
e117	0.0	0.0	1	0.0%
e122	1259.2	11938.2	1056	1.9%
e124	411.5	632.1	393	0.1%
e125	4684.3	11267.0	266	1.8%
e126	1.8	6.0	17	0.0%
e128	59.1	130.2	23	0.0%
e129	96.1	347.6	73	0.1%
e130	977.2	3625.0	164	0.6%
e139	49.7	99.1	153	0.0%
e141	126.9	443.7	124	0.1%
e145	31.5	155.9	23	0.0%
e148	67.5	92.6	132	0.0%
e149	553.2	3921.5	62	0.6%
e152	12299.3	21728.4	155	3.4%
e158	0.0	387.1	114	0.1%
e159	3.3	4.6	49	0.0%
e160	0.1	0.1	7	0.0%
e171	0.0	0.0	1	0.0%
e173	65.2	105.4	246	0.0%
e174	0.0	174.1	4	0.0%
e175	241.0	20277.8	522	3.2%
e179	0.1	0.1	1	0.0%
e184	65.8	1586.0	691	0.3%
e186	2287.7	6979.0	984	1.1%
e187	4.7	19.5	52	0.0%
e191	135.7	169.7	49	0.0%
e193	424.2	1480.1	113	0.2%

e199	458.1	786.9	204	0.1%
e201	63.8	147.8	67	0.0%
e203	50.6	446.6	336	0.1%
e205	100.0	140.6	31	0.0%
e208	31.0	66.1	66	0.0%
e210	11.1	19.2	25	0.0%
e211	0.8	1.0	28	0.0%
e215	1675.0	5186.4	412	0.8%
e216	303.9	4367.4	2415	0.7%
e217	570.4	1731.7	1331	0.3%
e218	13.8	126.0	202	0.0%
e219	70.0	290.7	12	0.1%
e224	3.6	76.4	34	0.0%
e225	84.2	106.3	37	0.0%
e227	7.9	9.9	35	0.0%
e228	153.8	192.3	32	0.0%
e230	57.8	200.9	158	0.0%
e231	0.0	0.0	12	0.0%
e234	0.0	2.9	10	0.0%
e238	0.0	0.0	2	0.0%
e239	0.0	0.0	5	0.0%
j01	3564.3	26250.3	836	4.2%
EPSRC Total	87419.3	331964.6	39246	52.4%
n01	15848.1	33387.8	3960	5.3%
n02	21621.4	37840.9	21417	6.0%
n03	9102.4	26200.7	3939	4.1%
n04	3387.7	6581.8	2997	1.0%
NERC Total	49959.6	104011.3	32313	16.4%
b10	0.0	0.2	82	0.0%
b14	0.0	36.2	21	0.0%
BBSRC Total	0.0	36.3	103	0.0%
p01	0.4	4.0	400	0.0%
STFC Total	0.4	4.0	400	0.0%
x01	1035.2	5069.0	2274	0.8%
External Total	1035.2	5069.0	2274	0.8%
d11	151.4	213.4	61	0.0%
d15	0.9	25.6	136	0.0%
d16	13.5	111.7	276	0.0%
d23	1.1	4.1	62	0.0%
d25	334.9	898.4	162	0.1%
d26	14.5	12.1	3	0.0%
d27	14.3	22.2	57	0.0%
d28	2430.6	9309.3	1559	1.5%
d30	85.2	111.4	66	0.0%
d32	8.5	12.2	401	0.0%
d34	17.7	14.9	417	0.0%
d35	0.0	0.1	5	0.0%
d37	57.6	951.3	1095	0.2%
d39	0.0	26.8	220	0.0%
Director's Time Total	3130.3	11717.9	4555	1.9%
pr1u0705	0.0	1.9	1	0.0%
pr1u0706	0.0	6592.1	121	1.0%
PRACE Total	0.0	6594.0	122	1.0%
Total	**143477.2**	**464603.6**	**81819**	**73.4%**

3.3 Helpdesk

A total of 1120 queries with a specified service metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	918	929	98.8%	97.0%
Admin queries finished in 1 day	848	859	98.7%	97.0%
Queries assigned in 30 min	1107	1115	99.3%	97.0%
Technical assessments in 10 days	14	15	93.3%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	556	49.6%
Admin	303	27.1%
In-depth	176	15.7%
Technical	70	6.3%
Technical assessment class-1	6	0.5%
Technical assessment class-2	9	0.8%

Queries by Category

Query Category	Queries	Percentage
New User	161	14.4%
3rd Party Software	110	9.8%
Set group quotas	96	8.6%
New Password	88	7.9%
Set user quotas	79	7.1%
Batch system and queues	65	5.8%
Access to HECToR	60	5.4%
None	54	4.8%
Disk, tapes, resources	53	4.7%
Compilers and system software	49	4.4%
User behaviour	41	3.7%
New Group	35	3.1%
Other	29	2.6%
Login, passwords and ssh	29	2.6%
Update account	28	2.5%
Make Reservation	25	2.2%
User programs	21	1.9%
Join Project	18	1.6%
SAFE	16	1.4%
Add to group	14	1.2%
Node Failure	10	0.9%
Static website	7	0.6%

Query Category	Queries	Percentage
Remove account	7	0.6%
Archive	6	0.5%
Courses	5	0.4%
Performance and scaling	4	0.4%
Network	4	0.4%
Create certificate	2	0.2%
Gpu	1	0.1%
Remove project	1	0.1%
Porting	1	0.1%
Delete from project	1	0.1%

Queries by Handler Category

Handlers	Total	Automatic	Technical Assessment	Admin	Technical	In-depth	%age
OSG	605	556		27	16	6	54.0%
Cray	48			5	17	26	4.3%
USL	354			270	36	48	31.6%
CSE	113		15	1	1	96	10.1%

3.3.1 Quality Tokens

A number of positive quality tokens were received in 4Q11. No negative tokens were received.

Project	Positive Tokens
e05	5
x01	10
Total	**15**

3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Oct-11	Nov-11	Dec-11	4Q11
Technology Reliability (%)	85.00%	98.50%	100.0	94.5	99.9	98.3
Technology MTBF (hours)	100	126.4	∞	732.0	732.0	1098.0
Technology Throughput, hours/year	7000	8367	8615	7102	8588	8609
Capability jobs completion rate	70%	90%	100.0%	100.0%	100.0%	100.0%
Non in-depth queries resolved within 1 day (%)	85%	97%	98.7%	99.0%	98.8%	98.6%
Number of SP FTEs	7.3	8.0	8.8	8.5	7.4	8.2
SP Serviceability (%)	80.00%	99.00%	100.0%	97.7%	100.0%	99.3%

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 (Class 1a listed first, followed by Class 1b, Class 2a, and Class 2b)							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Richard Blake	50,803.70	37,126.50	13,677.10
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969.90	80,691.10	403,141.50
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124	311,568.60	826,879.90
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257,748.20	9,829.20	247,919
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400	7,020.10	23,379.90
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1a	Dr Andreas M Kempf	1,300	297.3	1,002.70
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1a	Prof Kai Luo	3,650	0	3,650
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000	713.2	5,286.80
e108	Jet Flap Noise	EPSRC	Class1a	Dr Sergey Karabasov	49,684.50	14,546.30	35,138.20
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	140,110.30	58,022	82,026.30
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	65,000	35,985.30	28,933.90
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887.90	7,947.50	14,936.40
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168,324.80	13,576.50	154,638.30

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584	8,271.40	17,312.60
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000	1,167.90	5,832.10
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7,092.10	3,494	3,598.10
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500	1,076.20	6,423.80
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500	1,945.80	8,554.20
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350	3,401.50	12,948.50
e143	Numerical Investigation of Jet Noise	EPSRC	Class1a	Dr Anurag Agarwal	0	0	0
e144	Numerical Simulation of Rotating Stall and Surge	EPSRC	Class1a	Dr Mehdi Vahdati	1,266	0.3	1,265.70
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191.90	367.8	821.6
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082.50	46,650.60	21,431.90
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000	161.7	9,838.30
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	500	279.1	220.9
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3,816	11.8	3,804.20
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208.10	0.9	20,207.10
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69,895.50	0	69,895.50
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4,872	0	4,872
e175	Fine-Scale Turbulence	EPSRC	Class1a	Dr Richard D Sandberg	50,000	509.4	49,334.90

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000	705.7	86,294.30
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	0	8,640
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130,500	732	129,768
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000	6,033.10	333,966.90
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	40,000	18,772.50	21,172.40
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030.20	4.8	6,025.40
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40,500	4,413.10	36,086.90
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38,345	0	38,345
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim Biktashev	4,400	50.7	4,349.30
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5,000	0	5,000
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	0	25,857.60
e211	Dendrite simulation	EPSRC	Class1a	Dr Jiawei Mi	300	1.1	298.9
e226	Novel Vibrational Spectroscopic Techniques	EPSRC	Class1a	Dr Andrew D Burnett	1,032.30	0	1,032.30
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	4,918.30	153.8	4,764.50
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50,000	0	50,000

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	0	500
e42	Computational Combustion for Engineering Applications	EPSRC	Class1a	Prof Kai Luo	32,000	30,171.30	1,828.70
e63	UK Applied Aerodynamics Consortium 2	EPSRC	Class1a	Dr Nick Hills	30,925.30	31,172.70	-247.4
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000	49,791.10	208.9
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403.50	49,479.60	80,912.30
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521.80	34,613.20	7,908.50
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600	3,203.10	6,396.90
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088.60	3,763.70	4,324.90
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	360,100	262,295.30	96,860.70
e92	Dynamo Action In Compressible Convection	EPSRC	Class1a	Mr Paul Bushby	4,075	4,074.40	0.6
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71,990.70	16,059.20	55,838.70
e139	Scalability Optimization for Largescale in-silico Simulations	EPSRC	Class1b	Dr Gernot Plank	3,121.10	588.9	2,532.20
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800	245.1	4,554.90
e174	3D instabilities in two-layer flows	EPSRC	Class1b	Dr Prashant Valluri	9,243.40	551.8	8,691.60
e177	Amorphous structures of mirror coatings	EPSRC	Class1b	Dr Ian Maclaren	5,700.80	301	5,399.70
e193	Colloids in Cholesteric Liquid Crystals	EPSRC	Class1b	Dr Davide Marenduzzo	28,793.90	15,035.50	13,642.90
e205	Feasilibility study of fine sediment transport	EPSRC	Class1b	Dr Ming Li	3,000	129.6	2,870.40

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e214	MD Studies of Low Salinity Enhanced Oil Recovery Mechanisms	EPSRC	Class1b	Prof Peter Coveney	3,086.60	0	3,086.60
e215	GIPAW DFT Calculation of NMR Parameters in Rare Earth Materials	EPSRC	Class1b	Dr John V Hanna	8,170	2,962.60	5,178.40
e216	Self-organised Lipid layers on Mercury	EPSRC	Class1b	Dr Pietro Ballone	1,535	693.8	800
e217	Exploring a Conformational Switch in a Macromolecule	EPSRC	Class1b	Dr Philip Biggin	2,835.40	879.9	1,955.60
e218	Computational Electron Collison Experiments using 2DRMP	EPSRC	Class1b	Dr Penny Scott	1,449.60	20.7	1,428.90
e219	Gust generation modelling for aeronautical purposes	EPSRC	Class1b	Prof Oubay Hassan	1,620	1,108.50	511.5
e220	Study of interacting turbulent flames 2	EPSRC	Class1b	Dr N Swaminathan	16,920	0	16,920
e233	Lengthscale bridging of biophysical systems	EPSRC	Class1b	Prof Jason Crain	10,400.60	229.5	10,171.10
e234	Simulations of carbon electrodes with ionic electrolytes	EPSRC	Class1b	Prof. Paul A Madden	1,968.50	0	1,968.50
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105.40	866.8	238.5
e210	The Defect Chemistry of TiO2	EPSRC	Class2a	Prof Russell Howe	300	177.3	122.7
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	0	400
e222	Integrated Drug Delivery Systems	EPSRC	Class2a	Dr Charles Laughton	400	430.9	-30.9
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	36.1	363.9
e225	New Ru and Ir Chromophores for Solar Cell Devices	EPSRC	Class2a	Dr Paul Elliott	300	89.2	210.8
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50	46.4	3.6

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e230	Adsorption and Diffusion in Metal-Organic Frameworks	EPSRC	Class2a	Dr Ahmet Ozgur Yazaydin	400	163.8	223.5
e231	Rapid Alloy Solidification	EPSRC	Class2a	Prof Peter Jimack	400	0	400
e232	Flow field analysis around flap type wave energy devices	EPSRC	Class2a	Dr Matthew Folley	289.9	0	289.9
e235	Modelling offshore wind	EPSRC	Class2a	Prof Simon Watson	400	0	400
e236	Simulations of Optical Communications Systems	EPSRC	Class2a	Dr Marc Eberhard	400	0	400
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400	0	400
e238	Porting to CAF and Experiments on the Peppermint Application	EPSRC	Class2a	Dr Stephen Jarvis	400	0	400
e239	Optimum Collection and Conversion of Light into Energy	EPSRC	Class2a	Dr Robert Paton	400	0	400
e242	Study of the Green Fluorescent Protein Fluorophore	EPSRC	Class2a	Dr Garth Jones	400	0	400
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600	56.7	1,543.30
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	2.4	797.6
STFC Projects							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	10,002.70	666.3	9,336.40
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	156,545.50	114,578.30	29,650.80
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Grenville Lister	500,832.30	372,726.20	127,912.40
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	405,647	323,838.60	81,140.40

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	104,161.50	80,595	23,550.80
u01	Melting of MgSiO3 Perovskite	NERC	Early use	Prof John P Brodholt	11,000	11,018.40	-18.4
BBSRC Projects							
b08	Int BioSim	BBSRC	Class1a	Mr Mark M Sansom	866	910	-44
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000	1,393.90	606.1
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000	632.5	9,367.50
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	0	42,600
Director's Time							
d11	NAIS	Directors Time	Service	Prof Mark Ainsworth	10,000	1,221.70	8,778.30
d15	HPC-GAP	Directors Time	Service	Dr David Henty	102	2.7	99.3
d16	ETC	Directors Time	Service	Dr Lorna Smith	501	199.6	301.4
d23	TEXT FP7	Directors Time	Service	Dr Mark Bull	1,500	30.5	1,469.50
d25	Code Scaling	Directors Time	Service	Dr Ken Rice	51,500	6,571.20	44,928.80
d26	Guest Training Accounts	Directors Time	Service	Miss Elizabeth Sim	50	43.2	6.8
d27	RollsRoyce	Directors Time	Service	Mr Paul Graham	50	27.3	22.7

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
d30	PARTRAC	Directors Time	Service	Dr Mark Sawyer	200	86.4	113.6
d32	APOS-EU	Directors Time	Service	Dr Michele Weiland	1,000	124.6	875.4
d33	Mark Westwood's Project	Directors Time	Service	Mr Mark Westwood	100	8.9	91.1
d34	Msc 2011-2012	Directors Time	Service	Dr David Henty	1,000	17.7	982.3
d37	CRESTA	Directors Time	Service	Dr Lorna Smith	1,000	61.8	924.7
d38	Windfarm Simulation	Directors Time	Service	Mr Adrian Jackson	171	0	171
d39	NCSA access	Directors Time	Service	Mr Mark A Straka	1,000	52.1	947.9
External Projects							
t01	NIMES: New Improved Muds from Environmental Sources.	External	Service	Dr Chris Greenwell	4,113.70	4,245.40	-131.8
x05	FIOS	External	Service	Mr Davy Virdee	1,130.10	1,076.60	53.5
x01	HPC-Europa	External	Service	Dr Judy Hardy	25,564.80	15,928.40	9,608.80
x06	Rhymney	External	Service	Dr Mark Sawyer	4.5	0.1	4.4
x07	RSI	External	Service	Miss Elizabeth Sim	10	0	10
PRACE Projects							
pr1u0705	Tangrin	PRACE	Class1a	Dr Chris A Johnson	2,800	27.8	2,772.20
pr1u0706	SIVE-2	PRACE	Class1a	Dr Chris A Johnson	5,000	1,199.90	3,800.10