



# HECToR Quarterly Report

**Jan - Mar 2012**

## **1 Introduction**

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

## 2 Executive Summary

- The upgrade to Phase 3 came to a conclusion in 1Q12. The remaining 10 cabinets of Interlagos were installed on 18<sup>th</sup> January, with acceptance tests completed in early February.
- The official Phase3 launch event took place in February. The event was attended by a number of senior stakeholders from the UK Research Councils, the University of Edinburgh and the government. The event was also attended by the winner of EPSRC's HECToR Cabinet Design competition.
- XE6 utilisation in 1Q12 was 68%, compared to 73% in 4Q11. Further details are available in Section 3.2 of the report. Charging was suspended on Nov 7<sup>th</sup> when the system was downsized in readiness for the Phase3 upgrade. This remained disabled until 13<sup>th</sup> January.
- A new, discounted AU rate for Phase3 was implemented as of 1<sup>st</sup> March. In conjunction with the increase in overall capacity, the kilo-AU (kAU) was also introduced.
- There were 5 service failures in 1Q12 as opposed to 4 in 4Q11. There were three maintenance/acceptance test overruns, one job scheduling problem, and one upgrade 'hot swap' related issue. The overall MTBF decreased from 4Q11 from 549 to 439 hours.
- The volume of single node failures remained constant from the previous quarter despite the introduction of new hardware.
- The initial acceptance testing for the Tertiary Storage solution was completed in late March. Work will continue in 2Q12 to fully integrate the solution.

### 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	24	18	18
Failures	3	0	2

##### 3.1.1 Performance Statistics

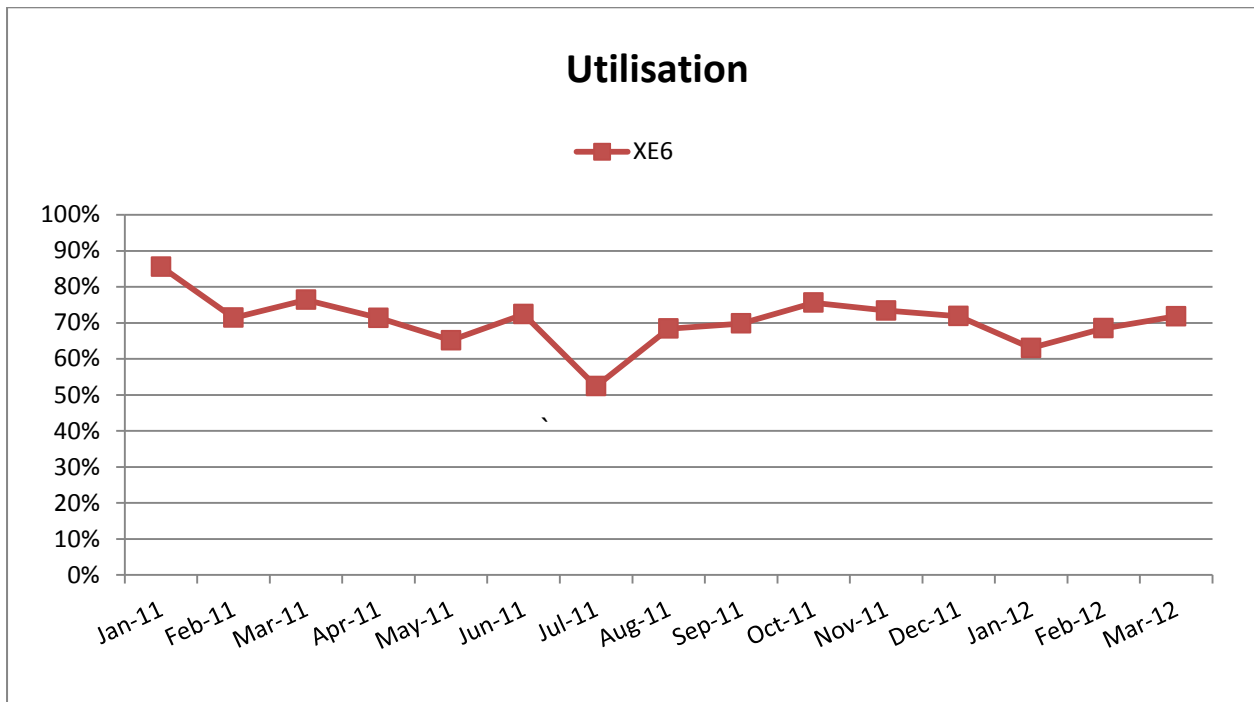
$MTBF = (732) / (\text{number of failures in a month})$

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

Attribution	Metric	Jan	Feb	Mar	Quarterly
Technology	Failures	3	0	2	5
	MTBF	244	∞	366	439
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	3	0	2	5
	MTBF	244	∞	366	439

## 3.2 HECToR Utilisation

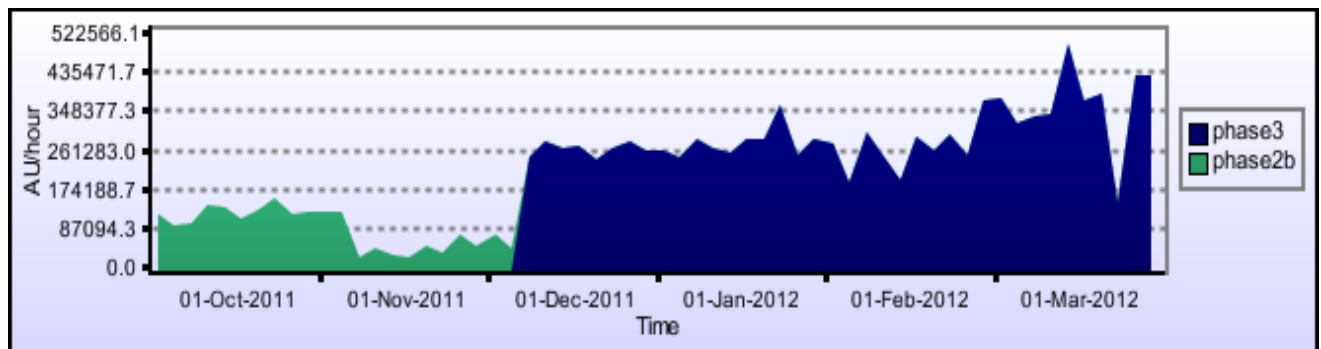
### 3.2.1 XE6 Utilisation



The XE6 utilisation quarterly average in 1Q12 was 67.9%, compared to 73% in 4Q11.

### Capability Usage

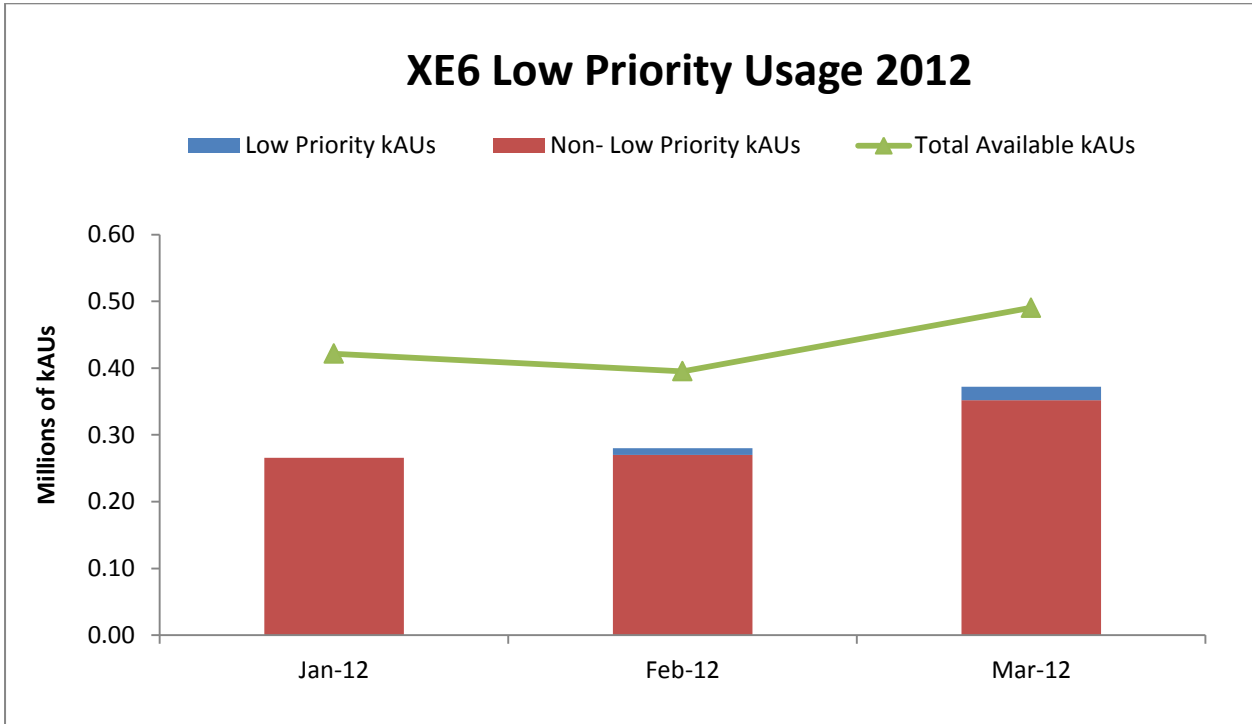
Capability usage has continued to trend upwards since the acceptance of the Phase3 system in January.



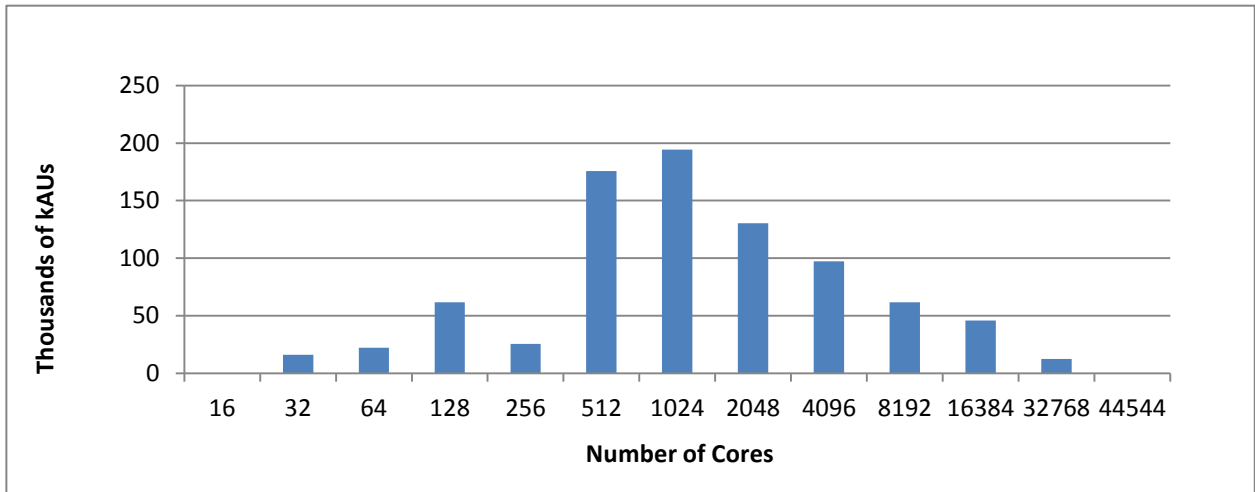
Raw AUs use by Machine of jobs using more than 511 CPUs

Low Priority Access

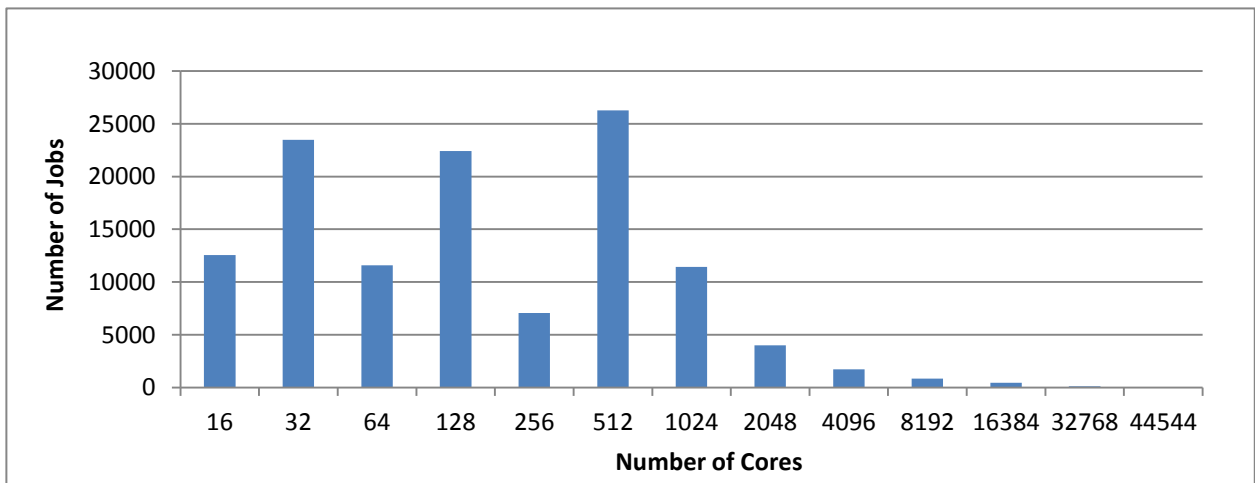
In 1Q12, low priority access accounted for 3.5% of the overall utilization.



### 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	0.00	10.20	68	0.0%
y02	1288.00	31797.30	254	2.4%
y03	324.80	558.60	1697	0.0%
y05	0.00	0.00	1	0.0%
y07	18.30	34.60	176	0.0%
z01	3664.60	5660.90	1226	0.4%
z03	786.70	1308.00	1111	0.1%
<b>Internal Total</b>	<b>6082.30</b>	<b>39369.50</b>	<b>4533</b>	<b>3.0%</b>
c01	2865.60	5069.80	2294	0.4%
e01	21364.90	40023.20	2420	3.1%
e05	143764.90	242875.90	27249	18.6%
e10	65.90	111.90	992	0.0%
e68	0.00	12.80	8	0.0%
e71	3365.50	5149.70	479	0.4%
e76	2049.70	2862.20	274	0.2%
e82	0.00	0.00	1	0.0%
e85	2523.10	3699.50	49	0.3%
e89	44511.20	80897.40	10654	6.2%
e104	430.60	677.00	694	0.1%
e107	7.60	3680.00	209	0.3%
e108	3911.70	6010.30	466	0.5%
e110	7497.00	13059.90	1039	1.0%
e122	23260.90	40211.30	1645	3.1%
e124	3845.70	15949.40	1299	1.2%
e125	7646.20	10865.00	422	0.8%
e126	3615.60	5231.50	178	0.4%
e127	269.70	419.40	44	0.0%
e128	109.40	136.90	17	0.0%
e129	608.30	840.00	122	0.1%
e130	398.70	560.60	123	0.0%
e139	170.70	214.40	119	0.0%
e141	617.80	961.70	366	0.1%
e145	20.50	32.40	46	0.0%
e149	1251.10	3942.80	31	0.3%
e158	145.00	216.40	122	0.0%
e159	12.60	20.90	243	0.0%
e160	0.70	1.30	18	0.0%
e173	48.00	74.50	187	0.0%
e174	104.40	285.90	7	0.0%
e175	775.20	13025.80	194	1.0%
e177	630.50	1050.10	313	0.1%
e179	1353.60	2159.90	116	0.2%
e184	544.40	1559.50	96	0.1%
e185	109.60	137.10	7	0.0%
e186	11403.70	17370.00	1511	1.3%
e187	384.10	566.00	620	0.0%
e193	5749.90	10107.00	534	0.8%
e203	699.40	1296.70	251	0.1%
e210	30.40	56.80	51	0.0%
e213	0.00	0.00	5	0.0%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
e214	2679.80	3351.00	310	0.3%
e215	4810.00	7419.40	465	0.6%
e216	1186.40	3038.50	991	0.2%
e217	1823.20	3013.70	784	0.2%
e218	310.70	394.40	139	0.0%
e219	0.00	58.00	1	0.0%
e220	2086.50	4643.20	44	0.4%
e224	376.40	593.80	149	0.1%
e225	53.60	99.70	38	0.0%
e228	0.00	0.00	11	0.0%
e229	1068.30	2135.90	398	0.2%
e230	448.30	837.60	207	0.1%
e231	191.60	400.40	161	0.0%
e232	82.60	132.00	99	0.0%
e233	7132.50	8937.80	1032	0.7%
e234	1065.60	1773.70	363	0.1%
e235	0.00	0.00	16	0.0%
e236	0.00	0.00	2	0.0%
e237	46.10	86.10	213	0.0%
e238	179.00	268.70	228	0.0%
e239	0.00	0.30	41	0.0%
e240	14.10	24.90	115	0.0%
e241	0.20	0.30	24	0.0%
e243	0.00	0.00	10	0.0%
e244	0.30	0.40	124	0.0%
j01	6786.70	15511.90	1225	1.2%
<b>EPSRC Total</b>	<b>326505.80</b>	<b>584144.40</b>	<b>62705</b>	<b>44.7%</b>
n01	33036.70	52311.60	3998	4.0%
n02	46126.30	78312.90	25722	6.0%
n03	43361.70	70652.50	5126	5.4%
n04	10386.20	17089.30	8782	1.3%
<b>NERC Total</b>	<b>132910.90</b>	<b>218366.30</b>	<b>43628</b>	<b>16.7%</b>
b14	66.70	107.40	120	0.0%
<b>BBSRC Total</b>	<b>66.70</b>	<b>107.40</b>	<b>120</b>	<b>0.0%</b>
p01	444.90	763.00	103	0.1%
<b>STFC Total</b>	<b>444.90</b>	<b>763.00</b>	<b>103</b>	<b>0.1%</b>
x01	5290.00	8913.40	3901	0.7%
x08	35.80	66.90	43	0.0%
<b>External Total</b>	<b>5325.80</b>	<b>8980.30</b>	<b>3944</b>	<b>0.7%</b>
d04	0.50	0.70	30	0.0%
d11	1225.60	1540.90	64	0.1%
d15	1.10	1.50	63	0.0%
d16	386.30	589.20	14	0.1%
d23	8.70	13.40	232	0.0%
d25	227.50	418.00	201	0.0%
d26	1.00	0.80	38	0.0%
d27	13.40	18.90	349	0.0%
d28	162.50	2014.70	858	0.2%
d29	0.60	1.00	27	0.0%
d30	38.80	48.60	35	0.0%
d32	14.20	26.50	398	0.0%
d34	37.10	50.90	544	0.0%
d37	959.20	2017.20	792	0.2%
d38	66.90	103.10	145	0.0%



Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
d39	799.90	1030.90	347	0.1%
d40	16.90	31.60	3	0.0%
d41	10743.00	14101.20	2503	1.1%
d42	0.10	0.20	4	0.0%
x07	0.40	0.40	12	0.0%
<b>DirectorsTime Total</b>	<b>14703.70</b>	<b>22009.70</b>	<b>6659</b>	<b>1.7%</b>
pr1u0704	1137.10	2060.80	102	0.2%
pr1u0705	1378.80	2243.70	170	0.2%
pr1u0706	5213.60	10215.10	175	0.8%
<b>PRACE Total</b>	<b>7729.50</b>	<b>14519.60</b>	<b>447</b>	<b>1.1%</b>
<b>Total</b>	<b>493769.50</b>	<b>888260.20</b>	<b>122139</b>	<b>67.9%</b>

### 3.3 Helpdesk

A total of 1252 queries with a specified service metric and 44 queries with no metric were completed in this period.

#### Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	1000	1009	99.1%	97.0%
Admin queries finished in 1 day	930	936	99.4%	97.0%
Queries assigned in 30 min	1236	1242	99.5%	97.0%
Technical assessments in 10 days	21	22	95.5%	97.0%

#### Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	586	46.81%
Admin	350	27.96%
In-depth	221	17.65%
Technical	73	5.83%
Technical assessment	22	1.76%

#### Queries by Category

Query Category	Queries	Percentage
New User	155	12.4%
New Password	140	11.2%
3rd Party Software	127	10.1%
Set user quotas	88	7.0%
Set group quotas	81	6.5%
Access to HECToR	76	6.1%
Compilers and system software	71	5.7%
Disk, tapes, resources	68	5.4%
Batch system and queues	59	4.7%

Query Category	Queries	Percentage
None	50	4.0%
User programs	40	3.2%
Login, passwords and ssh	34	2.7%
User behaviour	33	2.6%
Join Project	33	2.6%
Make Reservation	30	2.4%
New Group	25	2.0%
Other	22	1.8%
Courses	20	1.6%
Node Failure	18	1.4%
Update account	14	1.1%
SAFE	14	1.1%
Archive	14	1.1%
Static website	11	0.9%
Add to group	11	0.9%
Performance and scaling	4	0.3%
Remove account	3	0.2%
Delete from group	3	0.2%
Create certificate	3	0.2%
gpu	2	0.2%
Porting	2	0.2%
Grid	1	0.1%

### Queries by Handler Category

Handlers	Admin	In-depth	Technical	Automatic	TA	Total	%age
USL	300	41	48			389	31.1%
CSE	1	107	1		22	131	10.5%
OSG	48	6	14	586		654	52.2%
Cray	1	67	10			78	6.2%

### 3.3.1 Quality Tokens

A number of positive and negative quality tokens were received in 1Q12

Project	Positive Tokens	Negative Tokens
e232	0	1
e05	5	0
c01	0	3
<b>Total</b>	<b>5</b>	<b>4</b>

### 3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Jan-12	Feb-12	Mar-12	1Q12
Technology Reliability (%)	85.00%	98.50%	95.1%	100.0%	92.1%	95.6%
Technology MTBF (hours)	100	126.4	244.0	∞	366.0	439.2
Technology Throughput, hours/year	7000	8367	7651	8648	*7945	8082
Capability jobs completion rate	70%	90%	93.3%	100.0%	100%	97.8%
Non in-depth queries resolved within 1 day (%)	85%	97%	99.4%	98.9%	98.9%	99.1%
Number of SP FTEs	7.3	8.0	8.8	8.6	8.9	8.8
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

\*There were two service failures in March. One was due to a maintenance session overrun by 1 hour 45 min. The second failure was due to a PBS problem, which occurred on Saturday 24 March around 02:00 hours. The problem was cleared by 10:40 am next Monday morning. The reason for the long outage period in this case is that Cray are no longer on call during weekends or evenings. Work to resolve the issue waited until the Monday morning.

## **Appendix A: Terminology**

<b>TSL</b>	:	Threshold Service Level
<b>FSL</b>	:	Full Service Level
<b>SDT</b>	:	Scheduled Down Time
<b>UDT</b>	:	Unscheduled Down Time
<b>WCT</b>	:	Wall Clock Time
<b>MTBF</b>	:	Mean Time Between Failures = 732/Number of Failures
<b>SP</b>	:	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
<b>EPSRC Projects (Class 1a listed first, followed by Class 1b, Class 2a, and Class 2b)</b>							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Richard Blake	50,803.70	40,316.90	10,486.80
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969.90	100,858.70	382,973.90
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124.00	455,025.40	683,423.10
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257,748.20	9,908.40	247,839.80
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	50,000.00	49,791.10	208.9
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403.50	52,620.70	77,771.10
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521.80	36,542.50	5,979.30
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	303,698.00	96,402.00
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	7,464.10	22,935.90
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 Mesoscales to	EPSRC	Class1a	Prof Kai Luo	3,650.00	0	3,650.00
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000.00	720.6	5,279.40
e108	Jet Flap Noise	EPSRC	Class1a	Dr Sergey Karabasov	49,684.50	18,502.70	31,181.70
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	140,110.30	65,394.40	74,653.90
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	58,395.70	91,604.30
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887.90	12,231.40	10,648.50
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168,324.80	20,844.40	147,370.40
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584.00	11,887.00	13,697.00
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000.00	1,505.50	5,494.50
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7,092.10	3,603.50	3,488.70
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500.00	1,305.00	6,195.00
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500.00	2,340.20	8,159.80
e141	A numerical study of turbulent manoeuvring-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350.00	4,027.80	12,322.20
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	1,266.00	0.3	1,265.70
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191.90	390.8	798.6

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082.50	48,139.90	19,942.60
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000.00	161.7	9,838.30
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	24.4	3,791.60
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208.10	1.7	20,206.40
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	4,872.00	0	4,872.00
e175	Fine-Scale Turbulence	EPSRC	Class1a	Dr Richard D Sandberg	50,000.00	1,051.60	48,792.80
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000.00	2,059.30	84,940.70
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	732.4	129,767.60
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000.00	6,142.70	333,857.30
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70,000.00	29,821.70	40,178.30
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030.20	404.8	5,625.40
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

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim Biktashev	4,499.60	788.1	3,711.50
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5,000.00	0	5,000.00
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
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26,121.60	3,456.00	22,665.60
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	20,218.30	164.3	20,054.00
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50,000.00	1,176.60	48,823.40
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	0.2	499.8
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71,990.70	20,905.70	50,992.20
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105.40	866.8	238.5
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800.00	293.1	4,506.90
e174	3D instabilities in two-layer flows	EPSRC	Class1b	Dr Prashant Valluri	9,243.40	621.3	8,622.00
e177	Amorphous structures of mirror coatings	EPSRC	Class1b	Dr Ian Maclaren	5,700.80	1,026.60	4,674.20
e193	Colloids in Cholesteric Liquid Crystals	EPSRC	Class1b	Dr Davide Marenduzzo	28,793.90	21,066.90	7,611.60
e215	GIPAW DFT Calculation of NMR Parameters in Rare Earth Materials	EPSRC	Class1b	Dr John V Hanna	8,170.00	7,631.50	372.9



Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e233	Lengthscale bridging of biophysical systems	EPSRC	Class1b	Prof Jason Crain	10,400.60	7,138.50	3,262.10
e234	Simulations of carbon electrodes with ionic electrolytes	EPSRC	Class1b	Prof. Paul A Madden	1,968.50	1,138.70	829.8
e210	The Defect Chemistry of TiO <sub>2</sub>	EPSRC	Class2a	Prof Russell Howe	300	207.6	92.4
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	0	400
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	380	20
e225	New Ru and Ir Chromophores for Solar Cell Devices	EPSRC	Class2a	Dr Paul Elliott	300	150	150
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saxena	50	46.4	3.6
e230	Adsorption and Diffusion in Metal-Organic Frameworks	EPSRC	Class2a	Dr Ahmet Ozgur Yazaydin	400	506.1	-118.9
e231	Rapid Alloy Solidification	EPSRC	Class2a	Prof Peter Jimack	400	191.6	208.4
e232	Flow field analysis around flap type wave energy devices	EPSRC	Class2a	Dr Matthew Folley	289.9	88.6	201.2
e235	Modelling offshore wind	EPSRC	Class2a	Prof Simon Watson	400	0.6	399.4
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	60.4	339.6
e238	Porting to CAF and Experiments on the Peppermint Application	EPSRC	Class2a	Dr Stephen Jarvis	400	179	221
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

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e243	Tailored Structures for Orthopaedic Implantations	EPSRC	Class2a	Dr Carmen Torres-Sanchez	400	0	400
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	0	400
e248	Testing of a Distributed Coordinate Descent Method	EPSRC	Class2a	Dr Peter Richtarik	400	0	400
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600.00	56.7	1,543.30
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	14.1	785.9
e244	VOX-FE: Large Scale FE Bone Modelling on HECToR	EPSRC	Class2b	Prof Michael Fagan	800	0.3	799.7
e245	Parallelisation of a harmonic balance NS solver	EPSRC	Class2b	Dr Sergio Campobasso	800	0	800
<b>STFC Projects</b>							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	10,002.70	1,284.00	8,718.70
<b>NERC Projects</b>							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	166,545.50	147,484.40	19,061.10
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	dr grenville gms lister	494,832.30	419,178.70	75,653.60
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	405,647.00	367,984.70	36,994.20
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	104,161.50	90,478.40	13,634.40
<b>BBSRC Projects</b>							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000.00	1,393.90	606.1

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000.00	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	42,600.00	111.9	42,488.10
<b>Director's Time</b>							
d04	MSc in HPC	Directors Time	Service	Dr David Henty	613.5	477.2	136.3
d11	NAIS	Directors Time	Service	Prof Mark Ainsworth	10,000.00	2,438.30	7,561.70
d15	HPC-GAP	Directors Time	Service	Dr David Henty	102	3.9	98.2
d19	OpenFOAM Demo	Directors Time	Service	Dr Alan Gray	1,950.00	1,894.80	55.2
d21	GADGET	Directors Time	Service	Dr Adrian Jenkins	1,000.00	18.6	981.4
d23	TEXT FP7	Directors Time	Service	Dr Mark Bull	1,500.00	35.2	1,464.80
d24	SBSI	Directors Time	Service	Dr Stephen Gilmore	2,000.00	958.1	1,041.90
d25	Code Scaling	Directors Time	Service	Dr Ken Rice	51,500.00	6,803.70	44,696.30
d26	Guest Training Accounts	Directors Time	Service	Miss Elizabeth Sim	50	44.2	5.8
d27	Rolls	Directors Time	Service	Mr Paul Graham	50	40.7	9.3
d28	Simulations of antimicrobial peptides	Directors Time	Service	Dr Andrew R Turner	7,641.70	7,641.70	0
d29	Nu-FuSe	Directors	Service	Mr Adrian Jackson	500	0.9	499.1

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
		Time					
d30	PARTRAC	Directors Time	Service	Dr Mark Sawyer	200	124	76
d31	Semileptonic Decay	Directors Time	Service	Prof Richard Kenway	1,000.00	0	1,000.00
d32	APOS-EU	Directors Time	Service	Dr Michele Weiland	1,000.00	143.3	856.7
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	1,000.00	61.3	938.7
d35	PhD	Directors Time	Service	Dr Mark Bull	10	0	10
d36	Genome	Directors Time	Service	Dr Alan Gray	3,460.00	0	3,460.00
d37	CRESTA	Directors Time	Service	Dr Lorna Smith	11,000.00	1,117.20	9,882.80
d38	Windfarm Simulation	Directors Time	Service	Mr Adrian Jackson	171	81.1	89.9
d39	NCSA access	Directors Time	Service	Mr Mark A Straka	1,000.00	799.9	200.1
d40	Computational Chemistry at St Andrews	Directors Time	Service	Dr Herbert Fruchtl	2,000.00	16.9	1,983.10
d41	NPL Project	Directors Time	Service	Dr Ulrich Zachariae	45,000.00	10,898.00	34,102.00
d42	Oxford Nanopore Technologies	Directors Time	Service	Dr Jayne Wallace	400	0.1	399.9
<b>External Projects</b>							
t01	NIMES: New Improved Muds from Environmental Sources.	External	Class1a	Dr Chris Greenwell	4,113.70	4,245.40	-131.8

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
x01	HPC-Europa	External	Service	Dr Judy Hardy	38,762.40	21,209.10	17,553.30
x05	FIOS	External	Class1a	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
<b>PRACE Projects</b>							
pr1u0704	HIFLY	PRACE	Class1a	Dr Chris A Johnson	8,450.40	1,523.10	6,927.30
pr1u0705	TanGrin	PRACE	Class1a	Dr Chris A Johnson	14,084.00	1,516.20	12,567.80
pr1u0706	SIVE-2	PRACE	Class1a	Dr Chris A Johnson	14,000.00	5,213.60	8,786.40