



# HECToR Quarterly Report

January – March 2011

## 1 Introduction

This report covers the period from 1 January 2011 at 0800 to 1 April 2011 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/1Q11.php>

## 2 Executive Summary

- The Phase 2b system completed the Gemini Upgrade acceptance tests in January. The Phase 2b system became the contractual service as of 1st Feb 2011.
- Taking both Phase 2a and Phase 2b into consideration, the average utilisation in 1Q11 was 74%. Utilisation on the XE6 averaged 78% for the quarter. XT4 utilisation was 61%. Further details are available in Section 3.2 of the report.
- Reliability was greatly improved on the previous quarter. There were 5 service failures in 1Q11 as opposed to 9 in 4Q10. There were no service failures in March. Three of the failures were as a result of hardware faults on the Phase 2a system in January. The other two failures related to elements of the shared filesystem. The total MTBF increased over 3Q10 from 244 to 439 hours.
- The volume of single node failures remained low.
- The X2 Vector system was very reliable in 1Q11. Charging remained suspended on the X2, resulting in an overall utilisation of 36%, compared to 32% in 4Q10.
- The helpdesk statistics were again excellent. 20 positive quality tokens were received from users in 1Q11, with no negative tokens received.
- The NERC Large Memory Server (LMS) was installed and tested in February. A subset of NERC users has access to the server to perform post-processing activities.
- The HECToR GPGPU test-bed completed acceptance tests in March. Users from two EPSRC and one NERC consortia now have access to the facility.
- It has been confirmed that the Phase 2a system (both XT4 and X2) will be decommissioned as of 31<sup>st</sup> May 2011.
- High level plans for HECToR Phase 3 were announced in early April. The Phase 3 system will be based on an extension and upgrade of the current Cray XE6 system (Phase 2b). The solution supplied will be a 30 cabinet system utilising the next generation AMD Interlagos processor and Cray's Gemini interconnect. The machine will have a projected theoretical peak of 820TF and as such represents a greater than two-fold increase in capability over the current Phase 2b system
- Plans to re-introduce the original 592TB of lustre disk into esFS are currently being progressed. The high level plan is to configure a second separate esFS filesystem, rather than expand the existing esFS filesystem. Users would then have access to one of the two filesystems. A migration plan is being formulated to cause as little disruption as possible.

### 3 Quantitative Metrics

#### 3.1 Reliability

The metrics in Section 3.1 relate solely to the service machine – i.e. Phase 2a for January 2011 and Phase 2b for February and March.

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

	Jan	Feb	Mar
Incidents	16	16	18
Failures	3	2	0

##### 3.1.1 Performance Statistics

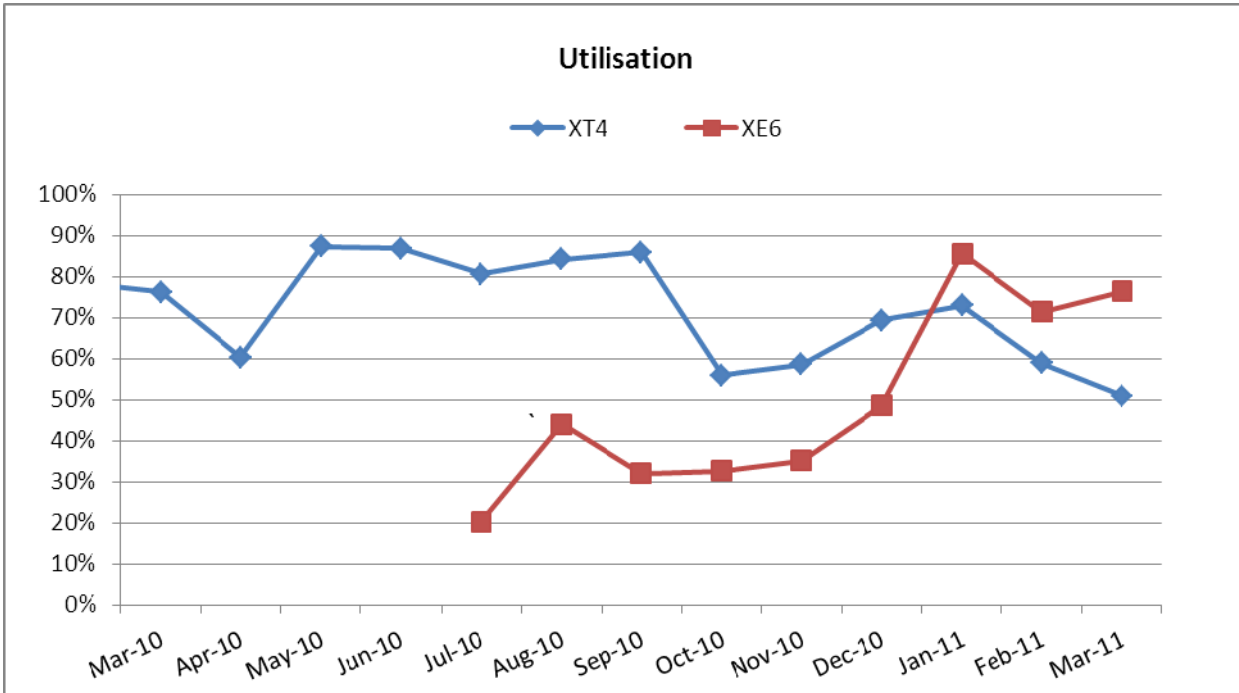
MTBF =  $(732)/(\text{number of failures in a month})$

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

Attribution	Metric	Jan	Feb	Mar	Quarterly
Technology	Failures	3	2	0	5
	MTBF	244	366	∞	439
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	3	2	5	9
	MTBF	244	366	∞	439

## 3.2 HECToR Utilisation

### 3.2.1 Overall Utilisation

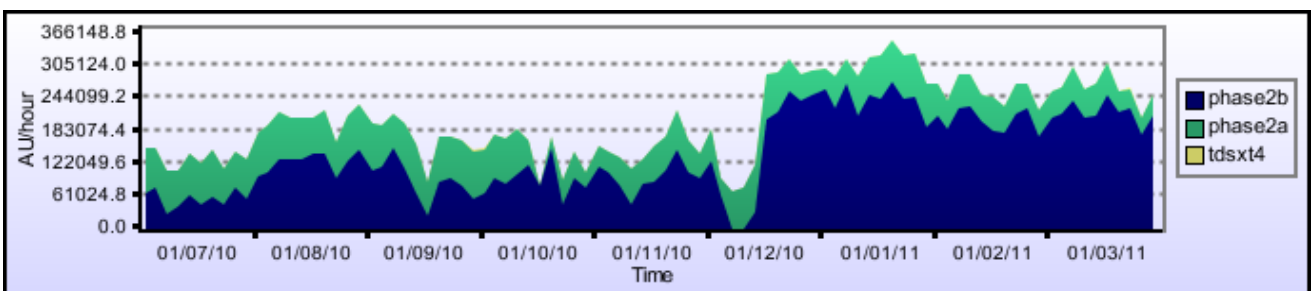


Taking both Phase 2a and Phase 2b into consideration, the average utilisation in 1Q11 was 74%.

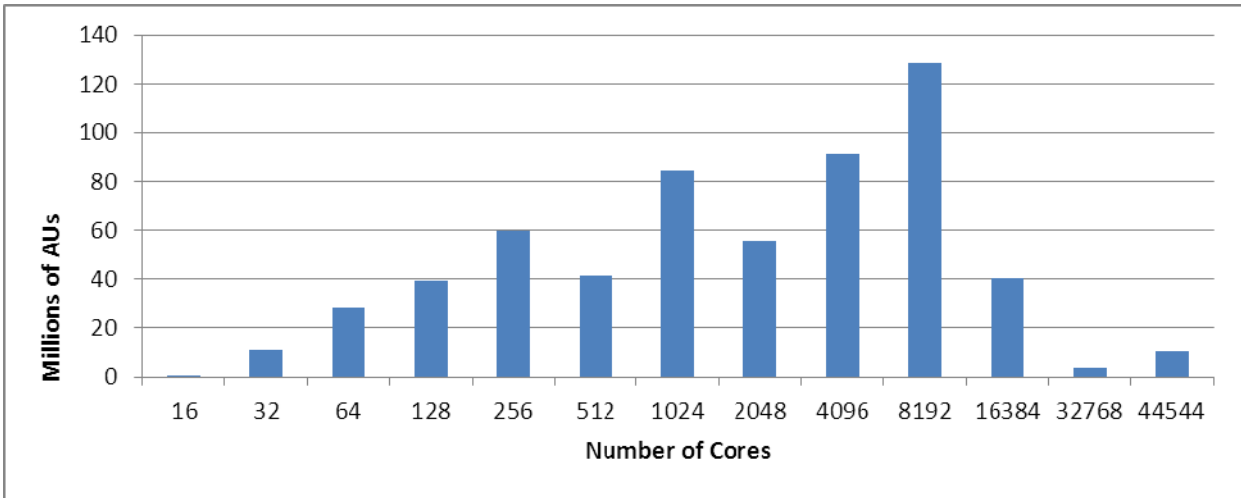
The Phase 2a utilisation quarterly average in 1Q11 was 61%, which was the same as the average in 4Q10. Utilisation on the Phase 2b system was 78% in 1Q11 as opposed to 39% in 4Q10. Charging was disabled on the Phase 2b system in January during the Gemini acceptance testing period.

The upgrade to Gemini has had a notable impact on the utilisation of the system. The AU usage on the respective systems can be seen below.

**AU Usage by Machine**



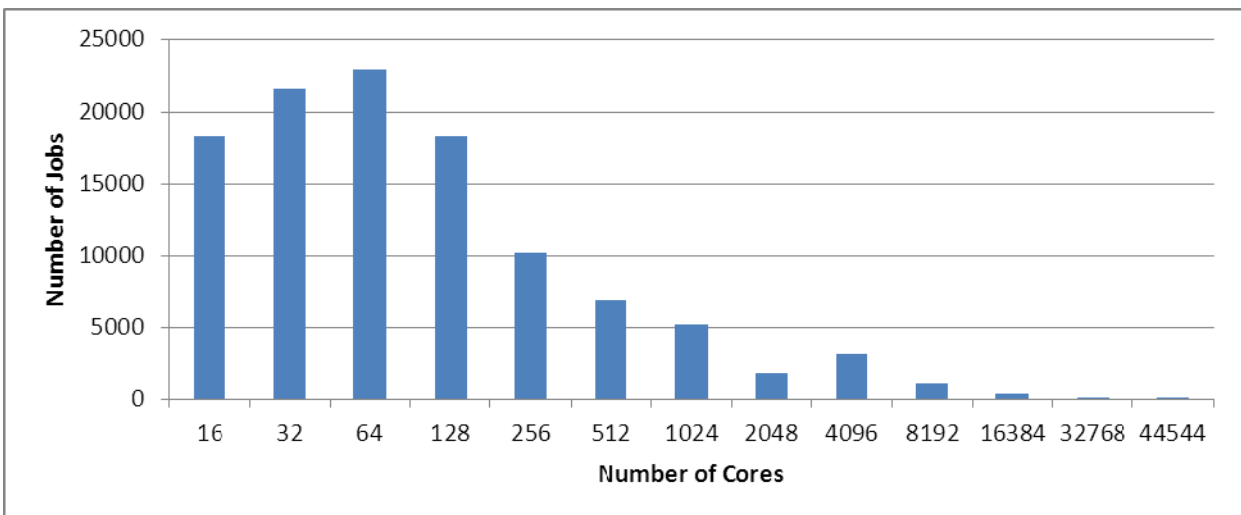
### 3.2.2 Job Size Analysis



The above graph shows the combined AU usage on Phase 2a and Phase 2b from January to April. The capability usage on the service is clearly demonstrated. Jobs in the range 4097 to 8192 cores accounted for 22% of the overall utilisation.

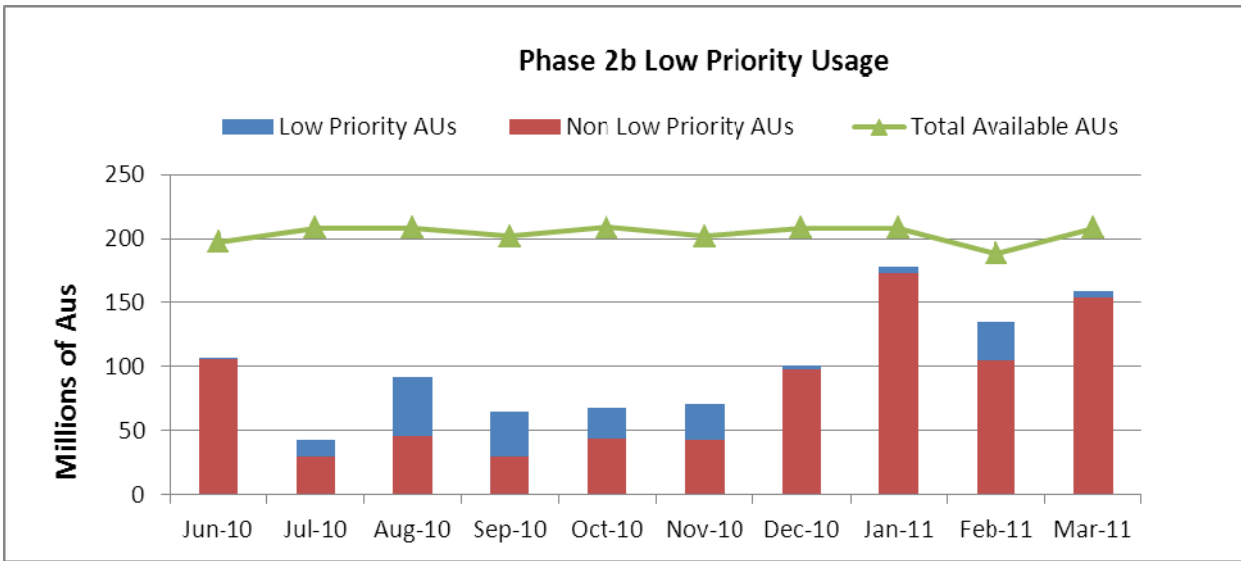
Comparing this to the graph below showing the number of jobs run in the same period, the jobs in the 8192 bracket accounted for just 1% of the total jobs. Utilisation of the service is driven by a modest number of users with the ability to run large jobs.

Looking at the number of jobs submitted in the period, the small jobs sizes clearly dominate the statistics. Jobs up to 256 Cores accounted for 83% of the jobs submitted, but only 23% of the overall utilisation.



### 3.2.3 Low Priority Access

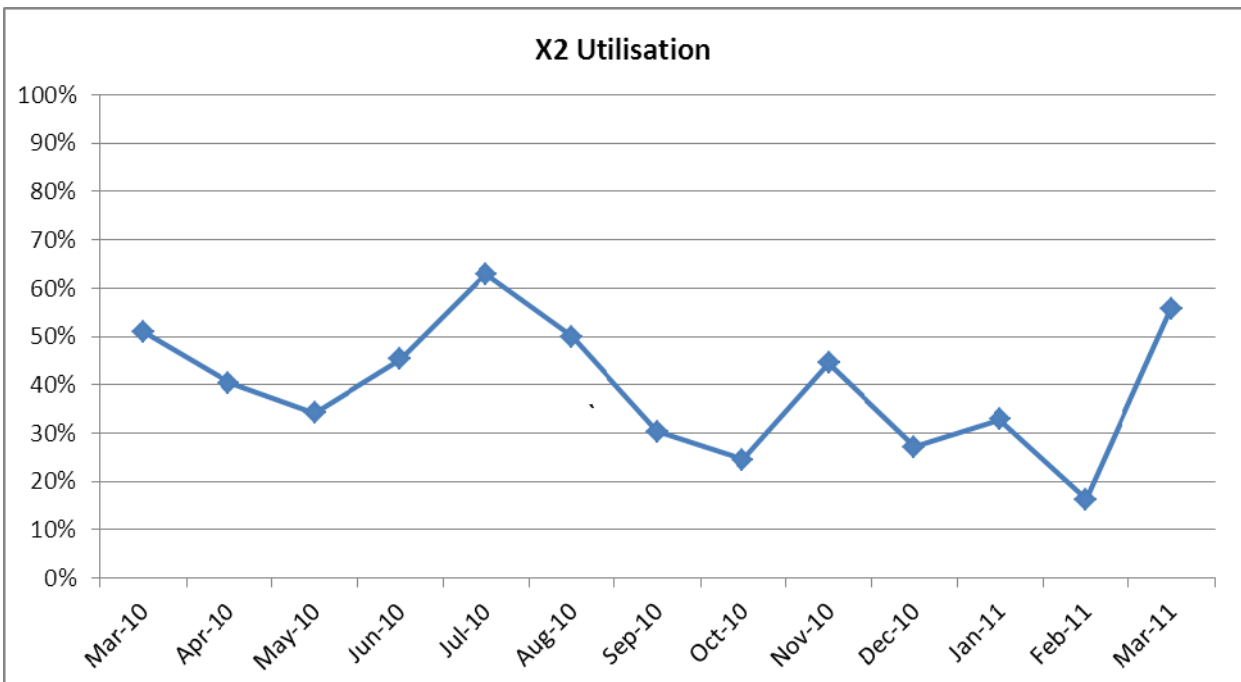
In 1Q11, low priority access accounted for 8.5% of the overall utilisation on the Phase 2b system.



Low Priority Access was disabled on the Phase 2a system in January when the Phase 2b system became the contractual service. In January, 2% of the utilisation on the Phase 2a system came from Low Priority Jobs.

### 3.2.4 X2 Utilisation

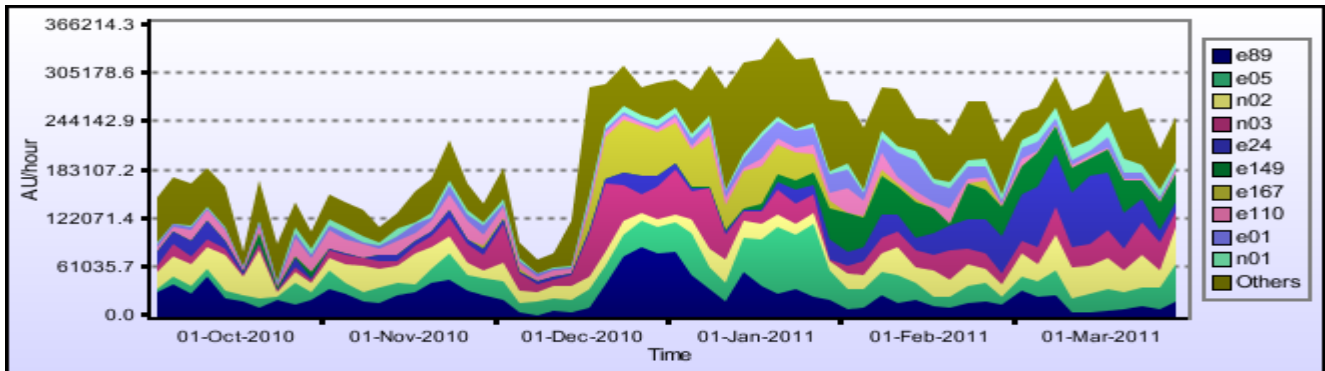
Accounting remained suspended on the X2 throughout 1Q11.



The overall X2 utilisation for 1Q11 was 36%. The X2 will be decommissioned after 31<sup>st</sup> May 2011.

### 3.2.5 Utilisation by Consortium

As below, a relatively small subset of projects contributes significantly to the overall utilisation.



The table below contains a summary of service utilisation by most active consortia. The full utilisation reports are available in the SAFE reports online at:

<http://www.hector.ac.uk/about-us/reports/quarterly/1Q11.php>

Project	phase2a (XT) %	phase2b (XT) %	phase2a (X2) %
y02	0.0%	1.7%	0.0%
z03	0.0%	0.4%	0.0%
<b>Internal Total</b>	<b>0.0%</b>	<b>2.1%</b>	<b>0.0%</b>
e149	0.0%	9.0%	0.0%
e05	8.9%	8.7%	18.2%
e89	2.3%	8.2%	0.0%
e24	11.6%	6.8%	0.0%
e167	0.0%	5.2%	0.0%
e124	0.0%	3.7%	0.0%
e01	4.3%	3.5%	17.4%
e110	2.0%	2.2%	0.0%
e108	0.3%	1.5%	0.0%
e193	0.0%	1.1%	0.0%
e82	0.0%	1.0%	0.0%
e190	0.0%	0.9%	0.0%
e196	0.0%	0.8%	0.0%
e68	0.6%	0.7%	0.0%
c01	0.3%	0.6%	0.0%
e85	0.0%	0.6%	0.0%
e92	0.0%	0.6%	0.0%
e122	0.0%	0.6%	0.0%
e192	0.0%	0.4%	0.0%
e170	0.2%	0.3%	0.0%
e117	0.0%	0.3%	0.0%
e10	0.3%	0.2%	0.0%
e107	0.3%	0.2%	0.0%
e125	0.0%	0.2%	0.0%
e141	0.0%	0.2%	0.0%
e188	0.0%	0.2%	0.0%
e186	2.5%	0.1%	0.0%

e71	0.9%	0.1%	0.0%
e70	0.0%	0.1%	0.0%
e76	0.0%	0.1%	0.0%
e84	0.0%	0.1%	0.0%
e127	0.0%	0.1%	0.0%
e128	0.0%	0.1%	0.0%
e194	0.0%	0.1%	0.0%
e195	0.0%	0.1%	0.0%
e63	3.8%	0.0%	0.0%
e104	1.0%	0.0%	0.0%
e191	0.8%	0.0%	0.0%
e185	0.6%	0.0%	0.0%
e42	0.1%	0.0%	0.0%
e146	0.1%	0.0%	0.0%
Others	0.3%	0.4%	0.0%
<b>EPSRC Total</b>	<b>41.2%</b>	<b>59.0%</b>	<b>35.6%</b>
n01	0.2%	2.9%	0.0%
n02	13.1%	4.5%	0.1%
n03	3.8%	8.1%	0.0%
n04	1.4%	1.0%	0.0%
<b>NERC Total</b>	<b>18.5%</b>	<b>16.5%</b>	<b>0.1%</b>
b10	0.1%	0.0%	0.0%
b100	0.0%	0.0%	0.0%
b12	0.0%	0.0%	0.0%
<b>BBSRC Total</b>	<b>0.1%</b>	<b>0.0%</b>	<b>0.0%</b>
p01	0.0%	0.0%	0.0%
<b>STFC Total</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>
x01	0.1%	0.2%	0.0%
<b>External Total</b>	<b>0.1%</b>	<b>0.2%</b>	<b>0.0%</b>
d03	0.0%	0.1%	0.0%
d25	1.0%	0.1%	0.0%
<b>Directors Time Total</b>	<b>1.0%</b>	<b>0.2%</b>	<b>0.0%</b>
<b>Overall Total</b>	<b>61.0%</b>	<b>78.0%</b>	<b>35.7%</b>



### 3.3 Helpdesk

A total of 1710 queries with a specified service metric were completed in this period. There were 46 queries without a metric completed in the same period.

#### Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	1401	1412	99.2%	97.0%
Admin queries finished in 1 day	1270	1278	99.4%	97.0%
Queries assigned in 30 min	1649	1655	99.6%	97.0%
Technical assessments in 10 days	17	19	91.7%	97.0%

#### Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	955	55.8%
Admin	323	18.9%
In-depth	233	13.6%
Technical	134	7.8%
No Metric	46	2.7%
Technical assessment	19	1.1%

#### Queries by Category

Query Category	Queries	Percentage
New Password	384	22.5%
New User	213	12.5%
Set user quotas	146	8.5%
3rd Party Software	115	6.7%
Disk, tapes, resources	104	6.1%
None	94	5.5%
Set group quotas	93	5.4%
Access to HECToR	77	4.5%
User behaviour	62	3.6%
Compilers and system software	61	3.6%
Batch system and queues	53	3.1%
User programs	38	2.2%
Node Failure	37	2.2%
Login, passwords and ssh	36	2.1%
Remove account	33	1.9%
Other	26	1.5%
Join Project	22	1.3%
Add to group	21	1.2%
SAFE	18	1.1%
Update account	17	1.0%
Courses	12	0.7%
New Group	8	0.5%
Archive	8	0.5%

Performance and scaling	7	0.4%
Create certificate	7	0.4%
Delete from group	6	0.4%
Static website	4	0.2%
Delete from project	4	0.2%
Network	2	0.1%
Porting	1	0.1%
Grid	1	0.1%

## Queries by Handler Category

Handlers	Auto	In-depth	Technical	Admin	Technical Assessment	Total	%age
OSG	954	16	39	35		1044	62.7%
Cray		47	10	2		59	3.5%
USL	1	60	84	285		430	25.8%
CSE		110	1	1	19	131	7.9%

### 3.3.1 Quality Tokens

A total of 20 positive quality tokens were set by users during 1Q11. No negative tokens were received.

Date	Tokens Awarded	Comment	Consortium
12/01/2011	*****	<i>Very fast reply to support request from helpdesk</i>	c01/e05/e117
17/01/2011	*****	Five positive tokens. No comment from the user	e05
27/01/2011	****	Four positive tokens. No comment from the user	d23
01/02/2011	****	Four positive tokens. No comment from the user	e05
23/02/2011	**	Two positive tokens. No comment from the user	e10/e24

### 3.4 Performance Metrics

All performance metrics relate to the service machine – i.e. Phase 2a for January 2011 and Phase 2b for February and March 2011.

Metric	TSL(%)	FSL(%)	Jan-11	Feb-11	Mar-11	1Q11
Technology reliability (%)	85.00%	98.50%	99.3	98.6	100.0	99.3
Technology MTBF (hours)	100	126.4	244.0	366.0	∞	439.2
Technology Throughput, hours/year	7000	8367	8625	8475	8648	8734
Capability jobs completion rate	70%	90%	100.0%	100.0%	100.0%	100.0%
Non in-depth queries resolved within 1 day (%)	85%	97%	100.0%	99.4%	98.7%	99.4%
Number of SP FTEs	7.3	8.0	8.2	8.3	9.4	8.6
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***

<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	AUs allocated	AUs used	AUs left
<b>EPSRC Projects</b>							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Richard Blake	50,803,723	30,394,889	20,408,834
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969,876	44,414,037	439,555,839
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124,000	165,092,263	973,971,737
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	122,748,188	8,516,691	114,231,497
e102	Numerical investigation of aerofoil noise	EPSRC	Class1a	Dr Richard D Sandberg	6,484,191	6,084,562	399,629
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400,000	4,344,652	26,055,348
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1a	Dr Andreas M Kempf	1,300,000	297,323	1,002,677
e106	Numerical Simulation of Multiphase Flow: From Mesoscales to	EPSRC	Class1a	Prof Kai Luo	3,650,000	0	3,650,000
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000,000	436,639	5,563,361
e108	Jet Flap Noise	EPSRC	Class1b	Dr Sergey Karabasov	7,684,524	7,584,758	99,766
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	49,100,000	40,717,532	8,382,468
e117	Biosurfactant via molecular dynamics simulations	EPSRC	Class1b	Dr Carmen Domene	18,889,069	13,173,249	5,715,819
e120	[dCSE] FF Transformations for plasma simulations	EPSRC	Class2b	Dr Colin M Roach	200,000	184,703	15,297
e121	[dCSE] Improving Performance using Wannier functions	EPSRC	Class1a	Prof Maria Merlyne DeSouza	2,680,305	2,299,591	380,714

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	65,000,000	21,319,060	43,680,940
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887,943	7,536,027	15,351,916
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	18,324,825	4,570,922	13,753,904
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584,000	4,288,531	21,295,469
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000,000	449,943	6,550,058
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	6,230,000	731,670	5,498,330
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500,000	599,444	6,900,557
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500,000	0	10,500,000
e131	Direct Simulation of a Pure Plume impinging on a density surface	EPSRC	Class2a	Dr Maarten van Reeuwijk	265,000	76,896	188,104
e133	Implementation of Established Algorithms to Extend HELIUM	EPSRC	Class2b	Prof Ken Taylor	800,000	0	800,000
e134	Numerical Simulation of Turbomachinery Flows	EPSRC	Class2a	Dr Francesco Montomoli	291,790	134,960	156,830
e135	DNS of unsteady turbulent flow over a smooth or a rough surface	EPSRC	Class2a	Dr Shuisheng He	204,000	174,763	29,237
e136	Modelling the UK Wind Power Resource	EPSRC	Class1b	Prof Gareth Harrison	5,679,268	4,996,068	683,200
e139	Scalability Optimization for Largescale in-silico Simulations	EPSRC	Class1b	Dr Gernot Plank	3,121,138	421,695	2,699,443
e141	A numerical study of turbulent manoeuvring-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350,000	764,119	15,585,881
e143	Numerical Investigation of Jet Noise	EPSRC	Class1a	Dr Anurag Agarwal	2	0	2
e144	Numerical Simulation of Rotating Stall and Surge	EPSRC	Class1a	Dr Mehdi Vahdati	1,266,001	325	1,265,676

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191,899	303,656	888,244
e147	Scale adaptive simulations of turbulent flows	EPSRC	Class2a	Prof Oubay Hassan	243,495	243,221	274
e148	Adding the molecular dynamics functionality to the quantum	EPSRC	Class2b	Prof Dario Alfe`	638,951	263,691	375,260
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082,500	44,263,624	23,818,876
e152	Turbulent entrainment	EPSRC	Class1b	Dr Maarten van Reeuwijk	22,212,628	7,212,628	15,000,000
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000,000	0	10,000,000
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600,000	1,203	1,598,797
e157	Global stability computations of separated flows	EPSRC	Class2a	Prof Jitesh S B Gajjar	299,996	68,960	231,036
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	500,000	5,331	494,669
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3,816,000	0	3,816,000
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208,060	0	20,208,060
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69,895,466	0	69,895,466
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4,872,000	0	4,872,000
e166	Large Eddy Simulation of LNG Pool Fires	EPSRC	Class2a	Dr Siaka Dembele	300,000	286,252	13,748
e167	LES of supersonic jets	EPSRC	Class1b	Prof William Dawes	2,696,000	2,608,238	87,762
e170	CFD Simulations of the BLOODHOUND SuperSonic Car	EPSRC	Class1b	Dr Ken Morgan	1,935,360	1,899,182	36,178
e171	Conformational switching of tetra-(bromophenyl) porphyrins	EPSRC	Class1b	Prof Mats Persson	3,289,521	1,767,735	1,521,786

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800,000	62,270	4,737,730
e174	3D instabilities in two-layer flows	EPSRC	Class2a	Dr Prashant Valluri	701,899	441,024	260,875
e175	Fine-Scale Turbulence	EPSRC	Class1a	Dr Richard D Sandberg	50,000,000	0	50,000,000
e176	Structure refinement of nanomaterials	EPSRC	Class2a	Prof. Peter G Bruce	300,000	0	300,000
e177	Amorphous structures of mirror coatings	EPSRC	Class2a	Dr Ian Maclaren	300,000	78,720	221,281
e178	Conformational changes in macromolecules	EPSRC	Class2a	Dr Philip Biggin	300,000	208,714	91,286
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000,000	0	87,000,000
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8,150,164	0	8,150,164
e183	Analysis of Processes in Hydrocarbon Fuel Droplets	EPSRC	Class1a	Prof Sergei Sazhin	8,640,000	0	8,640,000
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130,500,000	23,340	130,476,660
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000,000	1,289,361	338,710,639
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	40,000,000	6,335,880	33,664,120
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030,170	0	6,030,170
e188	Hydrostatic compression of energetic materials	EPSRC	Class1b	Prof Colin Pulham	2,000,000	1,108,863	891,137
e189	Towards Biomimetic Nanopores	EPSRC	Class1b	Mr Mark M Sansom	4,566,240	566,157	4,000,083
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1b	Prof Kenneth Badcock	3,500,000	1,846,750	1,653,251
e192	Physical properties of carbon nanotubes	EPSRC	Class1b	Dr Michael R C Hunt	2,534,400	1,784,097	750,304



Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e193	Colloids in Cholesteric Liquid Crystals	EPSRC	Class1b	Dr Davide Marenduzzo	12,500,000	4,000,256	8,499,744
e194	Direct Numerical Simulation of Meso-scale Combustor	EPSRC	Class1b	Dr N Swaminathan	3,701,520	1,179,242	2,522,278
e195	Sensitivity study of turbulence model	EPSRC	Class1b	Dr Alistair Revell	5,279,040	402,540	4,876,500
e196	Structure of intrinsically disordered proteins	EPSRC	Class1b	Dr Robert Best	3,600,000	3,599,557	443
e197	Potassium on graphite	EPSRC	Class2a	Dr Kai Hock	300,000	0	300,000
e198	Numerical Studies of Droplets	EPSRC	Class2a	Dr Kensuke Yokoi	300,000	0	300,000
e199	Microstructurally Faithful Modelling of Materials	EPSRC	Class2b	Dr Lee Margetts	800,000	1,466	798,534
e200	Late stage development of Richtmyer-Meshkov instability	EPSRC	Class2a	Prof Dimitris Drikakis	300,000	0	300,000
e201	Ab-initio modelling of cement and concrete	EPSRC	Class2a	Dr Davide Ceresoli	300,000	126	299,874
e205	Feasibility study of fine sediment transport	EPSRC	Class1b	Dr Ming Li	3,000,000	0	3,000,000
e24	DEISA	EPSRC	Class1a	Mrs Alison Kennedy	233,146,943	185,186,647	47,960,296
e35	Non-adiabatic processes	EPSRC	Class1a	Dr Tchavdar Todorov	12,246,862	4,164,267	8,082,595
e42	Computational Combustion for Engineering Applications	EPSRC	Class1a	Prof Kai Luo	32,000,001	30,171,317	1,828,684
e59	Turbulence in Breaking Gravity Waves	EPSRC	Class1a	Prof Ian P Castro	708,922	444,128	264,794
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000,000	47,981,003	2,018,997
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403,522	45,019,779	85,383,743
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521,798	34,076,186	8,445,612

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105,352	758,880	346,472
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600,000	3,203,118	6,396,882
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088,610	2,167,385	5,921,225
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	360,100,001	183,223,209	176,876,792
e92	Dynamo Action In Compressible Convection	EPSRC	Class1a	Mr Paul Bushby	4,075,000	3,143,550	931,450
y08	Testing	EPSRC	Early use	Dr David Jenkins	1,000	0	1,000
<b>STFC Projects</b>							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	3,020,000	557,361	2,462,639
<b>NERC Projects</b>							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Thomas Anderson	88,243,840	67,536,099	20,707,741
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Lois Steenman-Clark	399,286,988	262,959,220	136,327,768
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	328,158,215	258,389,252	69,768,963
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	105,712,967	69,415,096	36,297,871
<b>BBSRC Projects</b>							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000,000	1,393,875	606,125
b10	SPRINTing with HECToR [dCSE]	BBSRC	Class2b	Mr Terry Sloan	1,595,120	350,591	1,244,530
b12	Flu Analysis on HECToR	BBSRC	Class1a	Mr Adrian Jackson	50,000	0	50,000

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
b13	Linear Scaling DFT for Biochemistry Applications	BBSRC	Class1a	Dr David Bowler	5,587,200	0	5,587,200
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000,000	632,469	9,367,531
<b>Director's Time</b>							
d04	MSc in HPC	Directors Time	Service	Dr David Henty	343,500	205,163	138,337
d11	NAIS	Directors Time	Service	Prof Mark Ainsworth	10,000,001	366,859	9,633,143
d12	CoE HiGEM	Directors Time	Service	Dr Len L C Shaffrey	10,000,000	0	10,000,000
d13	CoE SENG	Directors Time	Service	Dr Stewart Cant	10,000,000	0	10,000,000
d15	HPC-GAP	Directors Time	Service	Dr David Henty	2,033	1,039	994
d16	ETC	Directors Time	Service	Dr Lorna Smith	501,000	154,897	346,103
d21	GADGET	Directors Time	Service	Dr Adrian Jenkins	1,000,001	18,584	981,417
d23	TEXT FP7	Directors Time	Service	Dr Mark Bull	1,500,000	17,145	1,482,855
d24	SBSI	Directors Time	Service	Dr Stephen Gilmore	2,000,000	958,106	1,041,894
d25	Code Scaling	Directors Time	Service	Dr Ken Rice	51,500,000	3,570,019	47,929,981
d26	Guest Training Accounts	Directors Time	Service	Miss Elizabeth Sim	50,000	13,922	36,079
d27	RollsRoyce	Directors Time	Service	Mr Paul Graham	50,000	0	50,000
d28	Simulations of antimicrobial peptides	Directors Time	Class1a	Dr Andrew R Turner	2,000,000	1,456	1,998,544
<b>External Projects</b>							

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e168	TEXT	External	Service	Dr Mark Bull	1,500,000	0	1,500,000
x01	HPC-Europa	External	Class1a	Dr Judy Hardy	16,415,790	9,808,272	6,607,518
x02	BlueArc (TDS)	External	Service	Mr M W Brown	1,000	0	1,000
x05	FIOS	External	Class1a	Mr Davy Virdee	1,130,100	1,076,575	53,525
x06	Rhymney	External	Service	Dr Mark Sawyer	4,500	23	4,477