



# HECToR Quarterly Report

Oct - Dec 2010

## 1 Introduction

This report covers the period from 1 October 2010 at 0800 to 1 Jan 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/4Q10.php>

## 2 Executive Summary

- 4Q10 was an extremely busy period for the service with two key improvements being implemented. During October and November all user data was transitioned to the new external lustre file-system 'esFS'. In December the XT6 was upgraded to include the Gemini interconnect. These were both significant improvements requiring two extended periods of disruption for users. A full review of these hardware changes will be included in the Annual Report.
- XT4 utilisation in 4Q10 was 61%, compared to 84% in 3Q10. Taking the 10-day downtime in October for esFS testing into consideration, the average utilisation was 68%. Further details are available in Section 3.2 of the report.
- Utilisation on the XT6 averaged 39% for the quarter. Charging on the XT6 was suspended on Dec 17<sup>th</sup> when the Gemini interconnect came online. This had a notable effect on the utilisation in the last two weeks of the quarter. Details are available in Section 3.2 of this report. Charging will be re-introduced on the completion of the acceptance testing and 10-day availability trials in late January.
- There were 9 service failures in 4Q10 as opposed to 7 in 3Q10. The overall MTBF decreased from 3Q10 from 314 to 244 hours. This still exceeds the full service level. A summary of all service failures will be included in the Annual Report.
- The volume of single node failures remained constant from the previous quarter.
- The Phase2b system was very reliable in 4Q10. There were 5 failures through October and November, and no failures in December. To date there have been no failures on the XE6 following the Gemini upgrade. Node failure rates were also low.
- The helpdesk statistics were again excellent. 13 positive and 9 negative quality tokens were received from users in 4Q10. An analysis is available in Section 3.3.1 of this report.
- The X2 Vector system was very reliable in 4Q10. Charging remained suspended on the X2, resulting in an overall utilisation of 31.9%, compared to 48.1% in 3Q10. Further details on X2 utilisation are available in Section 3.2.5. An analysis on overall X2 usage will also be included in the Annual Report.
- A review meeting was held with key HECToR user representatives on December 12<sup>th</sup>. A number of options for HECToR Phase 3 were presented and discussed. The options for Phase 3 will be further reviewed on 1<sup>st</sup> February by Cray, EPCC and EPSRC.

### 3 Quantitative Metrics

#### 3.1 Reliability

The metrics in Section 3.1 relate solely to the service machine – i.e. Phase 2a.

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

	<b>Oct</b>	<b>Nov</b>	<b>Dec</b>
Incidents	15	10	15
Failures	3	1	5

##### 3.1.1 Performance Statistics

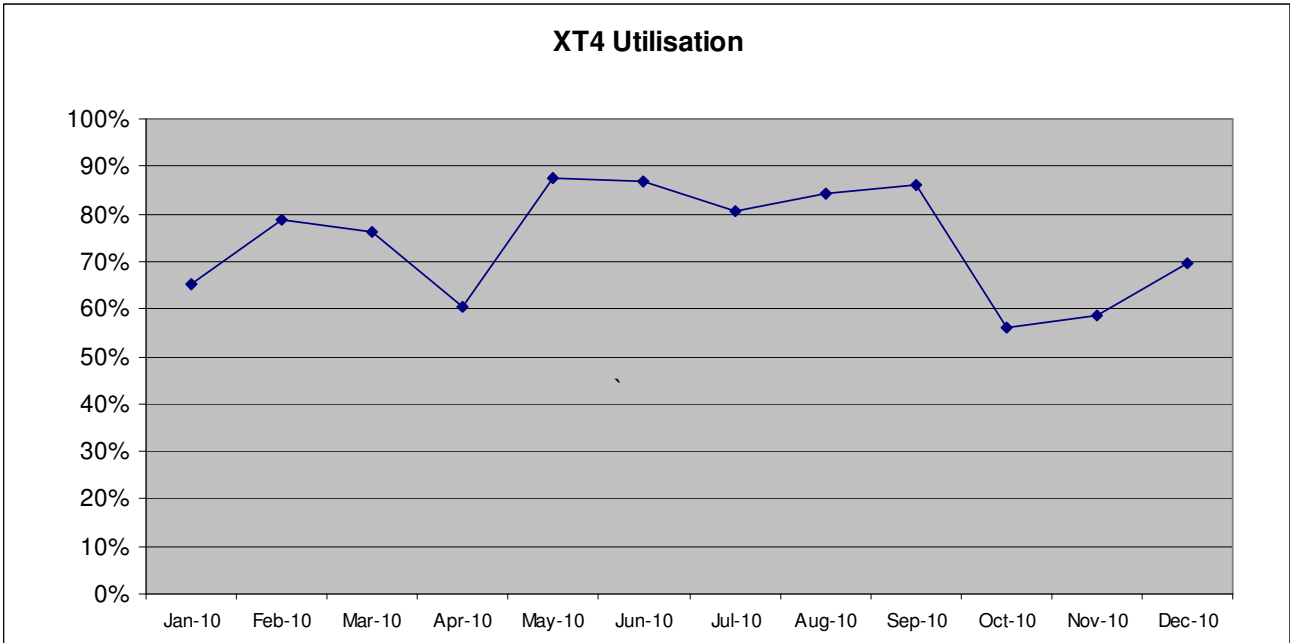
$MTBF = (732)/(\text{number of failures in a month})$

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

<b>Attribution</b>	<b>Metric</b>	<b>Oct</b>	<b>Nov</b>	<b>Dec</b>	<b>Quarterly</b>
Technology	Failures	3	1	5	9
	MTBF	244	732	146	244
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	3	1	5	9
	MTBF	<b>244</b>	<b>732</b>	<b>146</b>	<b>244</b>

## 3.2 HECToR Utilisation

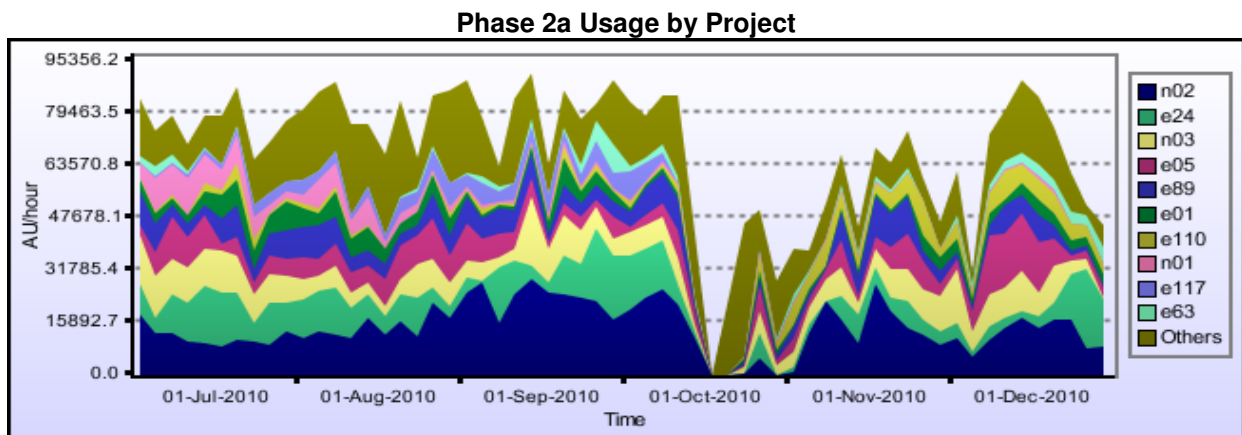
### 3.2.1 XT4 Utilisation



The XT4 utilisation quarterly average in 4Q10 was 61.3%, compared to 83.6% in 3Q10.

The steep drop in utilisation in October is partly due to the user disruption during the move to the esFS filesystem. The Phase2a service was unavailable to users to allow extensive Cray testing between 15th and 25th October. The migration of user data followed thereafter and this continued into November. During the migration of the data from Phase 2a to esFS, users were advised to use the Phase 2b service if possible to limit any risk of data corruption. If we discount the period in October when Phase2a was unavailable for users, the utilisation for that month changes from 56% to 76%.

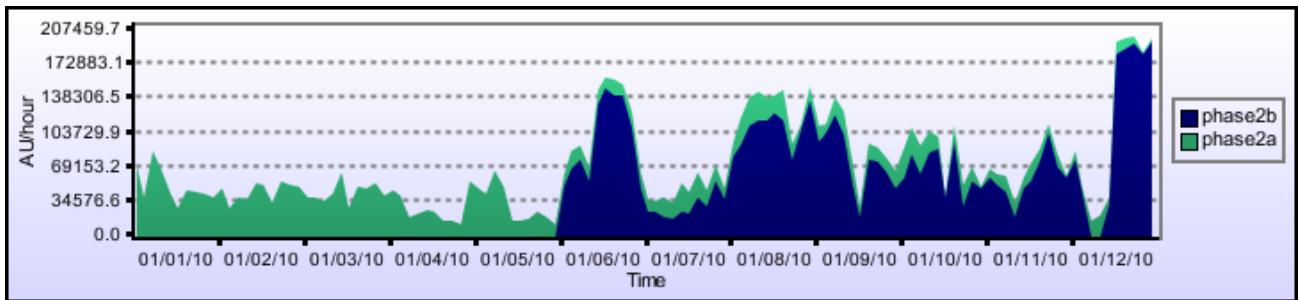
In addition to the impact of esFS, a number of the existing Class1b projects ended in September, and DEISA usage decreased slightly.



The utilisation of the Phase2a service started to recover in December.

## Capability Usage

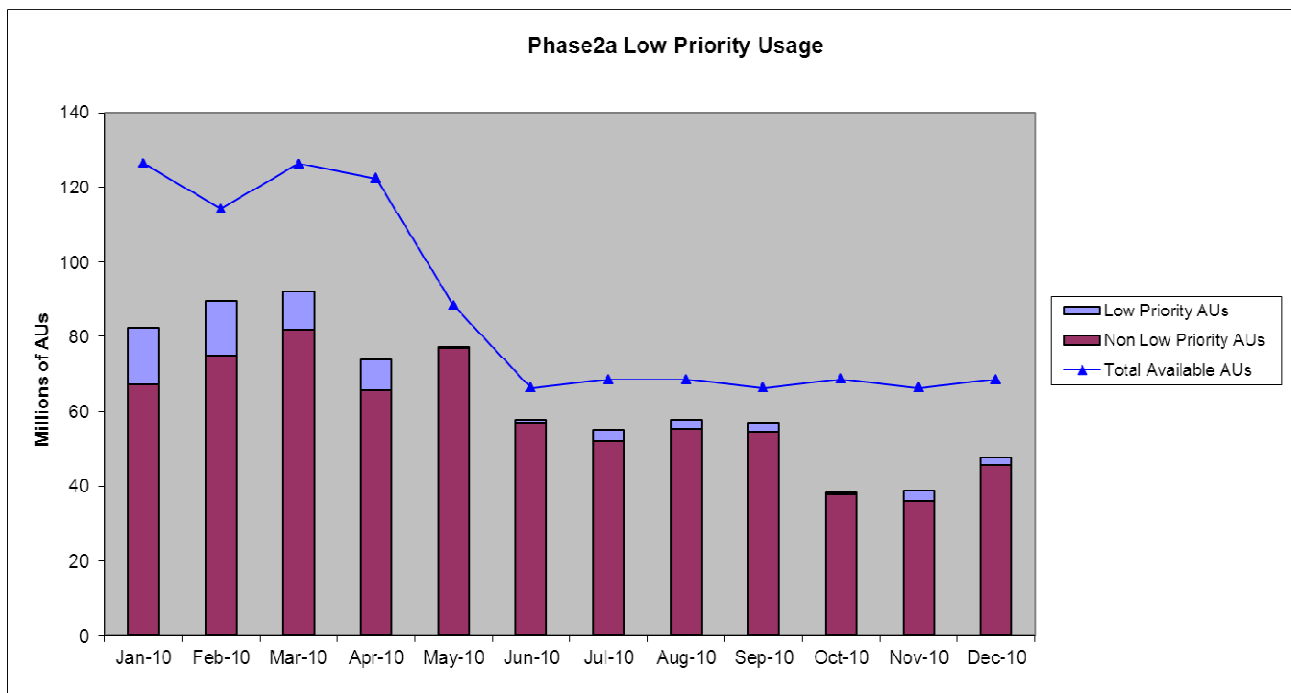
Capability usage has clearly increased with the arrival of the XT/E6.



The increase in December can be attributed to the suspension of charging on Phase2b when Gemini came online.

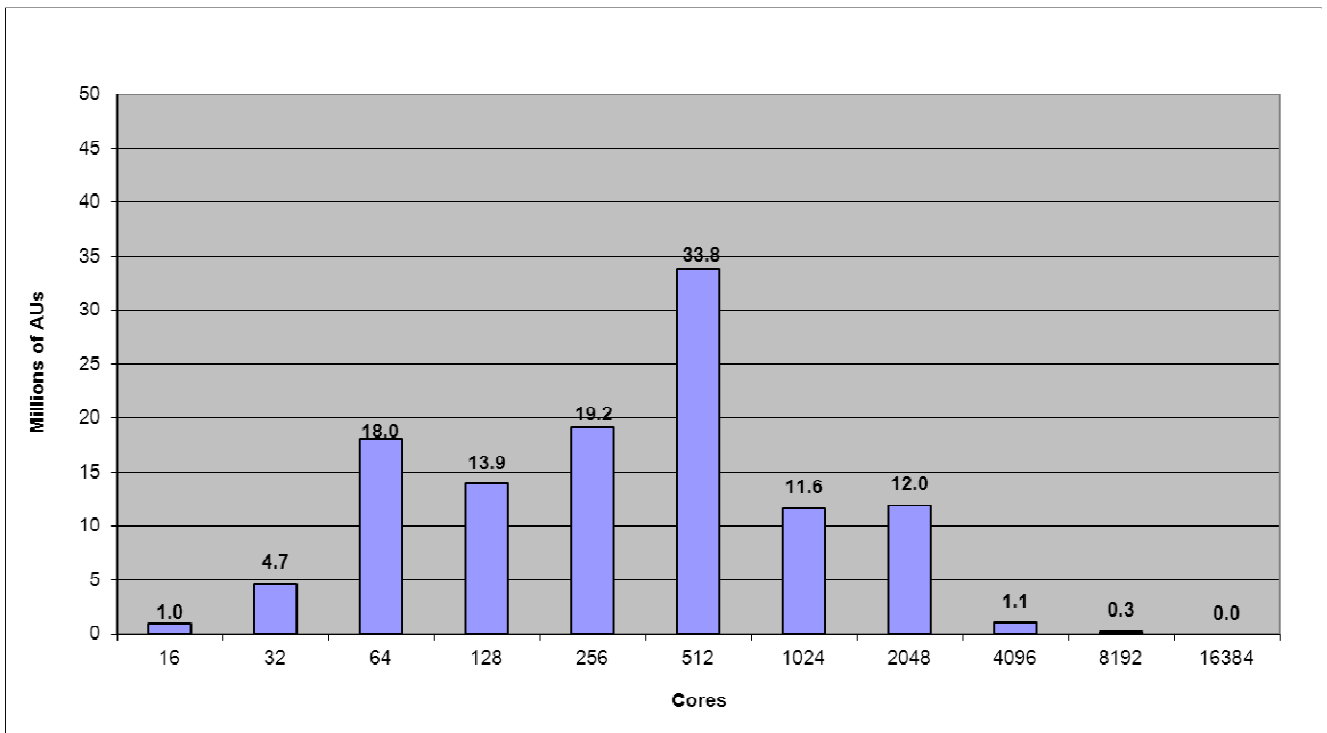
## Low Priority Access

In 4Q10, low priority access accounted for 4.1% of the overall utilisation on the XT4.

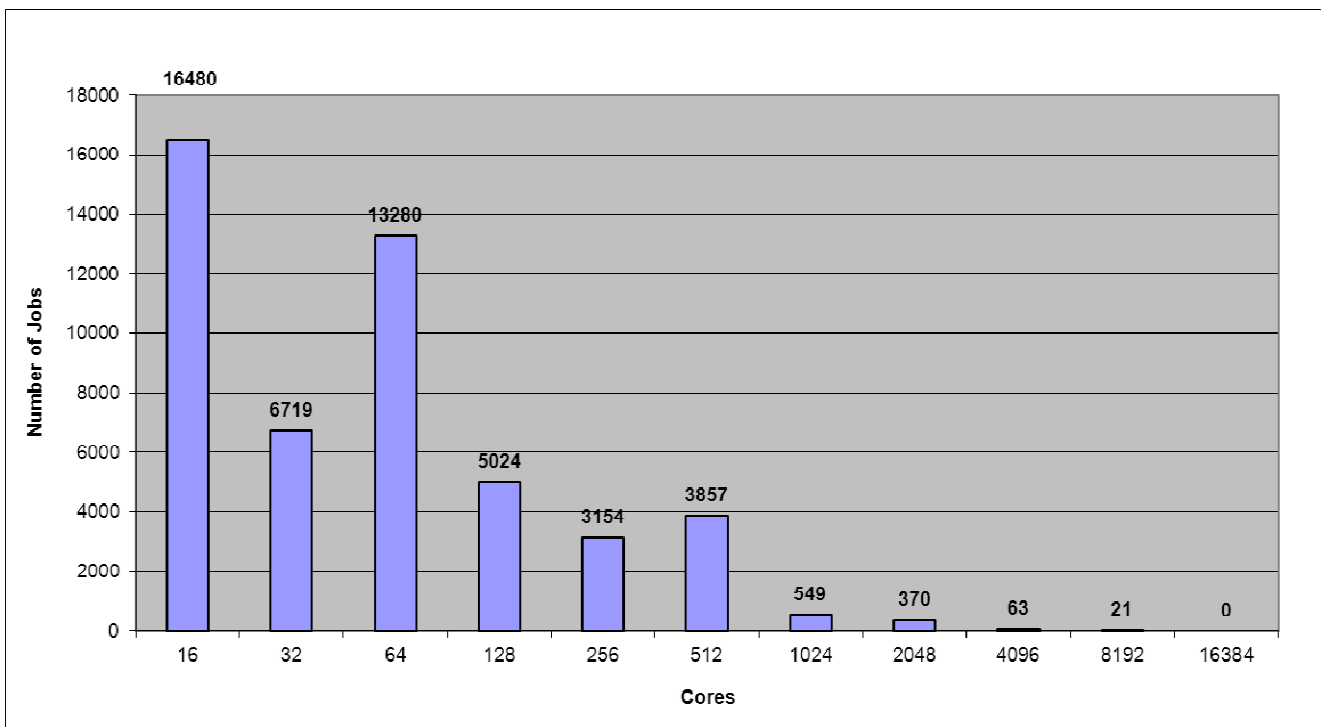


The low priority access mechanism works well and has not been abused by users. We would recommend that this remains in place.

### 3.2.2 XT4 Utilisation by Core Count

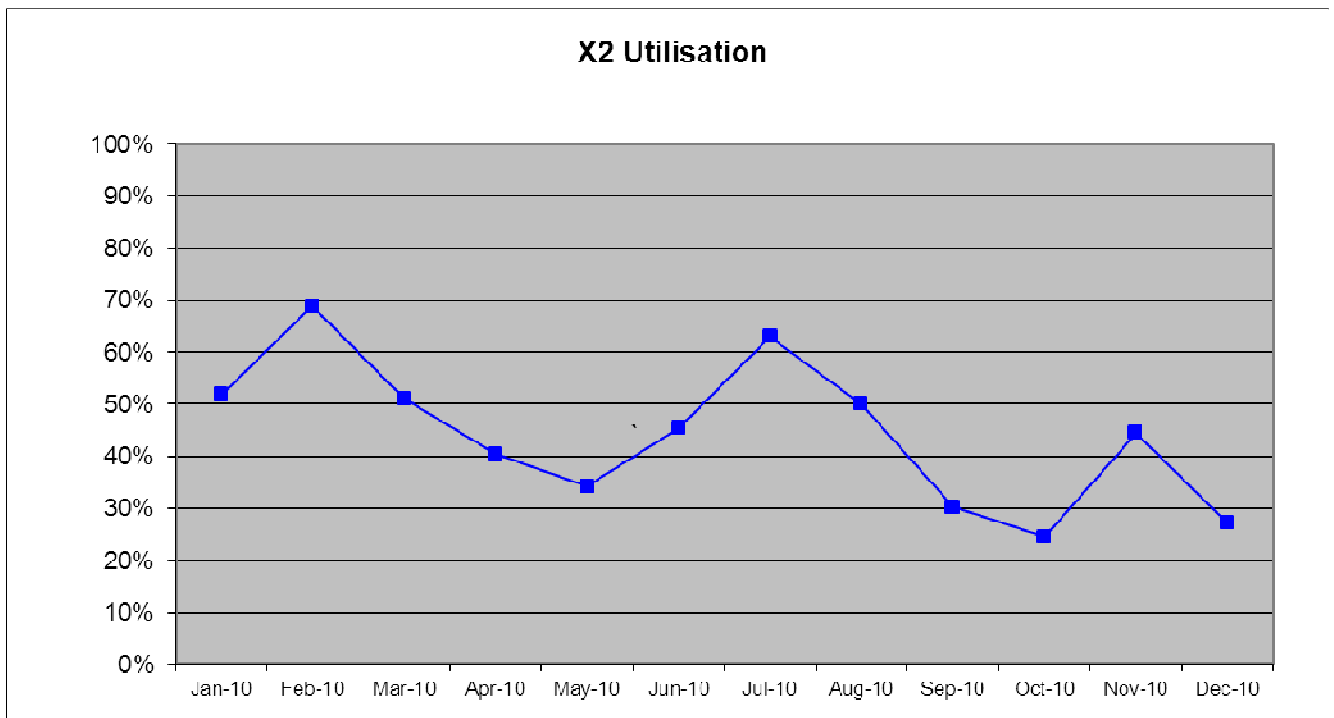


### 3.2.3 XT4 Number of jobs by Core Count



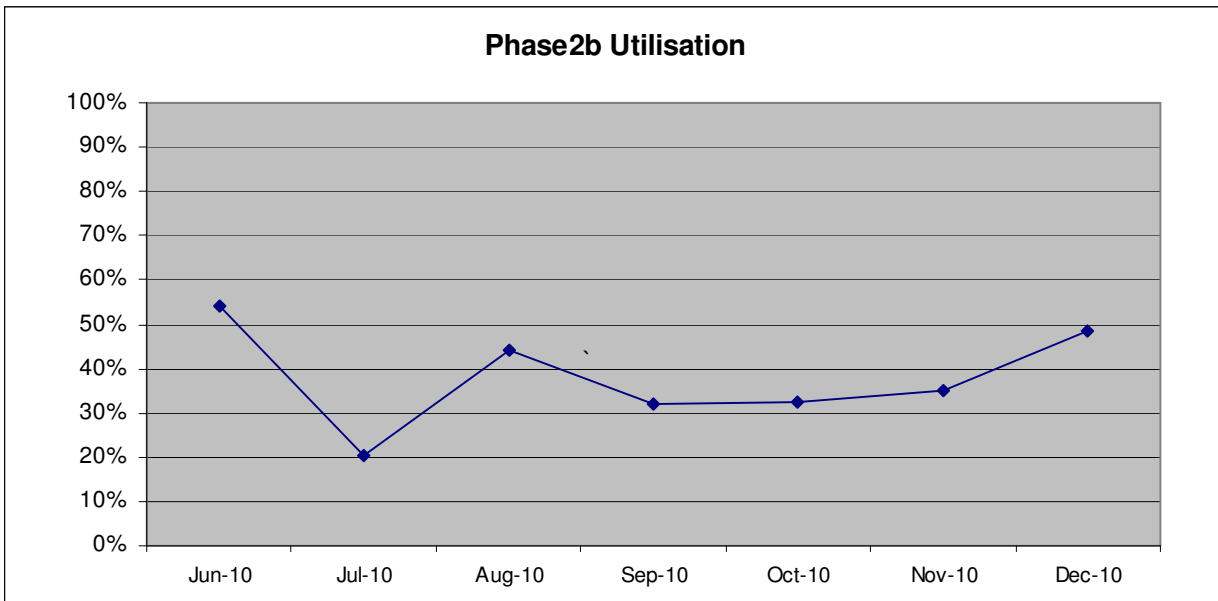
### 3.2.5 X2 Utilisation

Accounting remained suspended on the X2 throughout 4Q10.



The overall X2 utilisation for 4Q10 was 31.9%. Users of the X2 were contacted in 4Q10 regarding their use of the X2 in their research. The feedback from this will be included in the Annual Report.

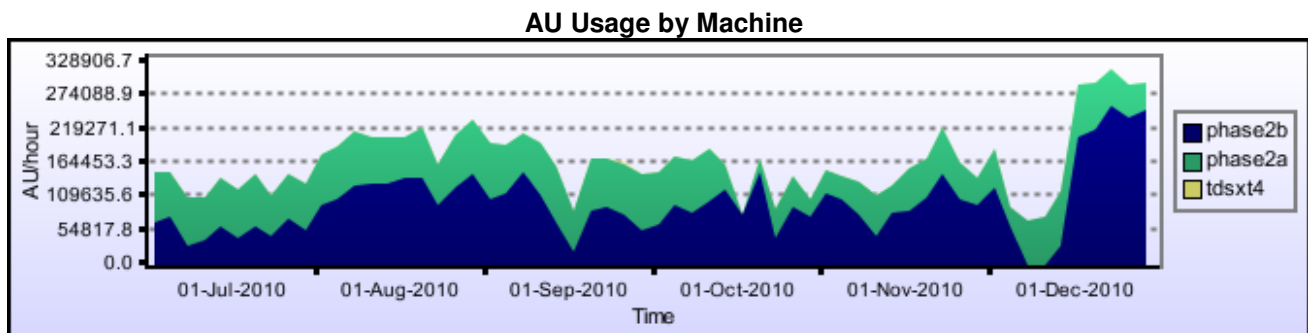
### 3.2.6 Phase 2b Utilisation



Utilisation on the Phase2b system was 39% in 4Q10 as opposed to 32% in 3Q10. The figures above do not take into account the downtime in December when the Gemini upgrade was taking place. The system was unavailable from Dec 6<sup>th</sup> to Dec 17<sup>th</sup>. Taking this into consideration, utilisation in December was 71% as opposed to 49%.

Charging was disabled on the XE6 when it went live with Gemini on 17<sup>th</sup> December. This has had a notable impact on utilisation.

As per the previous quarter; although the percentage utilisation on the Phase2b machine is lower than that on Phase2a, many more AUs were used on Phase2b.





### 3.2.4 Utilisation by Consortium

Project	XT4 Utilisation	XT6 Utilisation	X2 Utilisation
y01	0.6%	0.0%	0.0%
y02	1.6%	1.3%	0.0%
y03	0.0%	0.0%	0.0%
y04	0.0%	0.0%	0.0%
y06	0.0%	0.0%	0.0%
y07	0.0%	0.0%	0.0%
z01	0.1%	0.0%	0.0%
z02	0.0%	0.0%	0.0%
z03	0.0%	0.3%	0.0%
<b>Internal Total</b>	<b>2.3%</b>	<b>1.6%</b>	<b>0.0%</b>
c01	0.4%	0.5%	0.0%
e01	1.4%	0.9%	30.4%
e05	6.2%	4.0%	1.5%
e10	0.1%	0.0%	0.0%
e24	6.6%	0.6%	0.0%
e42	0.4%	0.0%	0.0%
e59	0.0%	0.0%	0.0%
e63	1.8%	0.3%	0.0%
e68	1.0%	0.2%	0.0%
e70	0.0%	0.0%	0.0%
e71	0.5%	0.0%	0.0%
e76	1.5%	0.0%	0.0%
e81	0.0%	0.0%	0.0%
e82	0.2%	0.9%	0.0%
e84	1.2%	0.0%	0.0%
e85	0.0%	1.0%	0.0%
e89	4.9%	9.4%	0.0%
e92	0.0%	0.6%	0.0%
e102	0.0%	0.0%	0.0%
e104	0.9%	0.0%	0.0%
e107	0.2%	0.0%	0.0%
e110	4.3%	2.6%	0.0%
e117	0.6%	0.0%	0.0%
e120	0.0%	0.0%	0.0%
e121	0.4%	0.0%	0.0%
e122	0.3%	0.4%	0.0%
e124	0.2%	0.3%	0.0%
e125	0.0%	0.0%	0.0%
e126	0.2%	0.0%	0.0%
e127	0.0%	0.0%	0.0%
e129	0.2%	0.0%	0.0%
e135	0.0%	0.0%	0.0%
e136	0.5%	0.3%	0.0%
e138	0.0%	0.0%	0.0%
e141	0.0%	0.4%	0.0%
e145	0.0%	0.0%	0.0%
e146	0.0%	0.0%	0.0%
e147	0.0%	0.0%	0.0%
e149	0.4%	0.2%	0.0%
e157	0.0%	0.0%	0.0%

Project	XT4 Utilisation	XT6 Utilisation	X2 Utilisation
e158	0.0%	0.0%	0.0%
e162	0.1%	0.0%	0.0%
e166	0.1%	0.0%	0.0%
e167	0.0%	3.2%	0.0%
e169	0.0%	0.0%	0.0%
e170	0.1%	0.0%	0.0%
e171	0.4%	0.1%	0.0%
e172	0.0%	0.0%	0.0%
e173	0.0%	0.0%	0.0%
e174	0.0%	0.0%	0.0%
e177	0.0%	0.0%	0.0%
e186	0.1%	0.0%	0.0%
e188	0.0%	0.8%	0.0%
e189	0.0%	0.0%	0.0%
e190	0.5%	0.1%	0.0%
e191	0.0%	0.0%	0.0%
e192	0.0%	0.1%	0.0%
e193	0.0%	0.0%	0.0%
e195	0.0%	0.0%	0.0%
e199	0.0%	0.0%	0.0%
<b>EPSRC Total</b>	<b>35.9%</b>	<b>27.2%</b>	<b>31.9%</b>
n01	0.4%	1.4%	0.0%
n02	13.7%	3.1%	0.0%
n03	7.0%	4.3%	0.0%
n04	0.4%	0.6%	0.0%
<b>NERC Total</b>	<b>21.5%</b>	<b>9.4%</b>	<b>0.0%</b>
b10	0.0%	0.0%	0.0%
<b>BBSRC Total</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>
p01	0.2%	0.0%	0.0%
<b>STFC Total</b>	<b>0.2%</b>	<b>0.0%</b>	<b>0.0%</b>
x01	0.4%	0.3%	0.0%
<b>External Total</b>	<b>0.4%</b>	<b>0.3%</b>	<b>0.0%</b>
d03	0.5%	0.0%	0.0%
d04	0.0%	0.0%	0.0%
d11	0.1%	0.0%	0.0%
d15	0.0%	0.0%	0.0%
d16	0.0%	0.0%	0.0%
d18	0.0%	0.0%	0.0%
d23	0.0%	0.0%	0.0%
d24	0.0%	0.3%	0.0%
d25	0.3%	0.0%	0.0%
<b>Directors Time Total</b>	<b>1.0%</b>	<b>0.3%</b>	<b>0.0%</b>
<b>Overall Total</b>	<b>61.3%</b>	<b>38.8%</b>	<b>31.9%</b>

### 3.3 Helpdesk

A total of 996 queries with a specified service metric were completed in this period.

#### Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	853	861	99.1%	97.0%
Admin queries finished in 1 day	795	800	99.4%	97.0%
Queries assigned in 30 min	979	980	99.9%	97.0%
Technical assessments in 10 days	23	24	95.8%	97.0%

#### Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	584	58.6%
Admin	216	21.7%
In-depth	111	11.1%
Technical	61	6.1%
Technical assessment class-1	22	2.2%
Technical assessment class-2	2	0.2%

#### Queries by Category

Query Category	Queries	Percentage
Set group quotas	129	13.0%
New User	127	12.8%
Set user quotas	113	11.3%
New Password	106	10.6%
None	68	6.8%
Disk, tapes, resources	47	4.7%
Access to HECToR	47	4.7%
3rd Party Software	42	4.2%
User behaviour	39	3.9%
Compilers and system software	34	3.4%
Add to group	34	3.4%
New Group	31	3.1%
Login, passwords and ssh	24	2.4%
Join Project	22	2.2%
User programs	21	2.1%
Other	20	2.0%
SAFE	19	1.9%
Batch system and queues	17	1.7%
Node Failure	15	1.5%
Update account	11	1.1%
Archive	6	0.6%
Create certificate	5	0.5%

Query Category	Queries	Percentage
Grid	4	0.4%
Remove account	3	0.3%
Performance and scaling	3	0.3%
Delete from group	3	0.3%
Courses	3	0.3%
Static website	2	0.2%
Network	1	0.1%

## Queries by Handler Category

Handlers	Total	Automatic	Technical Assessment	Admin	Technical	In-depth	%age
OSG	615	584		8	21	2	61.7%
CSE	84		24	1		59	8.4%
USL	262			207	29	26	26.3%
Cray	35				11	24	3.5%

### 3.3.1 Quality Tokens

A mix of positive and negative quality tokens were set by users during 4Q10.

The negative tokens related to known issues including system outages and file-system response times.

Positive tokens were received regarding the assistance given to new HECToR users, and also improvements seen in December with the arrival of the Gemini interconnect.

Project	Negative Tokens	Positive Tokens
e05	3	5
e82	1	4
n02	5	0
x01	0	4
<b>Total</b>	<b>9</b>	<b>13</b>

### 3.4 Performance Metrics

All performance metrics relate to the service machine – i.e. Phase 2a.

Metric	TSL(%)	FSL(%)	Oct-10	Nov-10	Dec-10	4Q10
Technology reliability (%)	85.00%	98.50%	87.6%	99.4%	93.8%	94.3%
Technology MTBF (hours)	100	126.4	244.0	732.0	146.4	204.3
Technology Throughput, hours/year	7000	8367	5116	8665	8088	7290
Capability jobs completion rate	70%	90%	94.3%	92.9%	100.0%	95.7%
Non in-depth queries resolved within 1 day (%)	85%	97%	99.3%	99.5%	98.2%	99.0%
Number of SP FTEs	7.3	8.0	8.1	9.0	7.6	8.2
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

## ***Appendix A: Terminology***

<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	30,803,723	27,861,147	2,942,576
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969,876	31,356,628	452,613,248
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124,000	122,237,924	1,016,826,076
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	10,248,188	7,104,643	3,143,545
e24	DEISA	EPSRC	Class1a	Mrs Alison Kennedy	233,146,943	126,052,911	107,094,032
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	30,021,151	1,978,850
e59	Turbulence in Breaking Gravity Waves	EPSRC	Class1a	Prof Ian P Castro	708,922	444,128	264,794
e63	UK Applied Aerodynamics Consortium 2	EPSRC	Class1a	Dr Nick Hills	30,925,323	25,925,815	4,999,508
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000,000	44,023,414	5,976,586
e70	Computation of Electron Transfer Properties	EPSRC	Class1a	Dr Jochen Blumberger	1,160,000	1,154,405	5,595
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403,522	42,731,053	87,672,469
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521,798	33,457,247	9,064,551
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105,352	682,588	422,764

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600,000	2,808,979	6,791,021
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088,610	2,122,745	5,965,865
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	360,100,001	161,367,725	198,732,276
e92	Dynamo Action In Compressible Convection	EPSRC	Class1a	Mr Paul Bushby	4,075,000	2,073,069	2,001,931
e102	Numerical investigation of aerofoil noise	EPSRC	Class1a	Dr Richard D Sandberg	6,484,191	6,084,516	399,675
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400,000	2,678,248	27,721,752
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	338,197	5,661,803
e108	Unsteady Propeller Noise	EPSRC	Class1b	Dr Sergey Karabasov	7,684,524	158,100	7,526,424
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	39,100,000	33,090,759	6,009,241
e117	Biosurfactant via molecular dynamics simulations	EPSRC	Class1b	Dr Carmen Domene	18,889,068	12,289,508	6,599,560
e120	[dCSE] FF Transformations for plasma simulations	EPSRC	Class2b	Dr Colin M Roach	200,000	170,213	29,787
e121	[dCSE] Improving Performance using Wannier functions	EPSRC	Class1a	Prof Maria Merlyne DeSouza	2,680,305	2,299,591	380,714
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	65,000,000	19,901,902	45,098,098
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887,943	6,248,060	16,639,883
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	18,324,825	3,572,645	14,752,180



Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	9,984,000	4,214,261	5,769,739
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000,000	17,041	6,982,959
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	6,230,000	0	6,230,000
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500,000	599,443	6,900,557
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500,000	0	10,500,000
e133	Implementation of Established Algorithms to Extend HELIUM	EPSRC	Class2b	Prof Ken Taylor	800,000	0	800,000
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	Dr Gareth Harrison	5,679,268	4,959,825	719,443
e141	A numerical study of turbulent manoeuvring-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350,000	166,810	16,183,190
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	24	1,265,977
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191,899	270,364	921,535
e146	G protein-coupled receptor dynamics	EPSRC	Class2a	Dr Irina Tikhonova	199,680	3,276	196,404
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	51,920,000	3,464,960	48,455,040
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000,000	0	10,000,000

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600,000	1,063	1,598,937
e157	Global stability computations of separated flows	EPSRC	Class2a	Prof Jitesh S B Gajjar	299,996	98	299,898
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	500,000	0	500,000
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	597,293	2,098,707
e170	CFD Simulations of the BLOODHOUND SuperSonic Car	EPSRC	Class1b	Dr Ken Morgan	1,935,360	256,728	1,678,632
e171	Conformational switching of tetra-(bromophenyl) porphyrins	EPSRC	Class1b	Prof Mats Persson	3,289,521	1,734,321	1,555,200
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800,000	49,092	4,750,908
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	0	300,000
e178	Conformational changes in macromolecules	EPSRC	Class2a	Dr Philip Biggin	300,000	208,714	91,286

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
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	0	130,500,000
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000,000	3,840	339,996,160
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	40,000,000	105,722	39,894,278
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	16,030,170	0	16,030,170
e188	Hydrostatic compression of energetic materials	EPSRC	Class1b	Prof Colin Pulham	2,000,000	246,199	1,753,801
e189	Towards Biomimetic Nanopores	EPSRC	Class1b	Mr Mark M Sansom	4,566,240	3,353	4,562,887
e19	Edinburgh Soft Matter and Statistical Physics Group	EPSRC	Class1a	Prof Michael Cates	4,663	6,171	-1,508
e190	Design of helicopter rotors	EPSRC	Class1b	Dr George N Barakos	4,500,000	1,193,384	3,306,616
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1b	Prof Kenneth Badcock	3,500,000	75,378	3,424,622
e192	Physical properties of carbon nanotubes	EPSRC	Class1b	Dr Michael R C Hunt	2,534,400	0	2,534,400
e193	Colloids in Cholesteric Liquid Crystals	EPSRC	Class1b	Dr Davide Marenduzzo	12,500,000	0	12,500,000
e194	Direct Numerical Simulation of Meso-scale Combustor	EPSRC	Class1b	Dr N Swaminathan	3,701,520	0	3,701,520
e195	Sensitivity study of turbulence model	EPSRC	Class1b	Dr Alistair Revell	5,279,040	4,618	5,274,422
e196	Structure of intrinsically disordered proteins	EPSRC	Class1b	Dr Robert Best	3,600,000	3	3,599,997

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
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	230	799,770
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	557,149	2,462,851
<b>NERC Projects</b>							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Thomas Anderson	89,243,840	53,343,347	35,900,493
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Lois Steenman-Clark	273,768,327	220,858,164	52,910,163
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	284,142,416	224,198,697	59,943,719
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	88,202,935	62,311,628	25,891,307
u01	Melting of MgSiO <sub>3</sub> Perovskite	NERC	Early use	Prof John P Brodholt	11,000,000	11,018,423	-18,423
<b>BBSRC Projects</b>							
b08	Int BioSim	BBSRC	Class1a	Mr Mark M Sansom	866,000	909,998	-43,998
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2,000,000	1,393,875	606,125
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000,000	632,465	9,367,535
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	HECToR Allocation	BBSRC	Class1a	Dr David Bowler	5,587,200	0	5,587,200
b10	SPRINTing with HECToR [dCSE]	BBSRC	Class2b	Mr Terry Sloan	795,120	61,996	733,124
<b>Director's Time</b>							
d03	EUFORIA	Directors Time	Service	Mr Adrian Jackson	2,400,000	2,426,575	-26,575
d04	MSc in HPC	Directors Time	Service	Dr David Henty	343,500	204,567	138,933
d11	NAIS	Directors Time	Service	Prof Mark Ainsworth	416,668	201,939	214,729
d12	CoE HiGEM	Directors Time	Service	Dr Len L C Shaffrey	10,000,000	0	10,000,000
d13	CoE SENG A	Directors Time	Service	Dr Stewart Cant	10,000,000	0	10,000,000
d14	CoE HiPSTAR	Directors Time	Service	Dr Richard D Sandberg	2,000,000	2,264,689	-264,689
d15	HPC-GAP	Directors Time	Service	Dr David Henty	2,033	1,038	995
d16	ETC	Directors Time	Service	Dr Lorna Smith	501,000	154,897	346,103
d17	CAF Optimisation	Directors Time	Service	Dr Jason Beech-Brandt	2	0	2
d18	FireGrid HPC	Directors Time	Service	Prof Arthur S Trew	600,001	251,409	348,592
d19	OpenFOAM Demo	Directors Time	Service	Dr Alan Gray	950,000	396,957	553,043
d20	CSCS	Directors Time	Service	Dr Alan Gray	50,000	0	50,000
d21	GADGET	Directors Time	Service	Dr Adrian Jenkins	1,000,001	18,584	981,417
d22	Summer Science Exhibition	Directors Time	Service	Prof. Angelos Michaelides	70,000	35,572	34,428

Code	Project Title	Funding Body	Class	Principal Investigator	AUs allocated	AUs used	AUs left
d23	TEXT FP7	Directors Time	Service	Dr Mark Bull	1,500,000	15,441	1,484,559
d24	SBSI	Directors Time	Service	Dr Stephen Gilmore	2,000,000	957,651	1,042,349
d25	Code Scaling	Directors Time	Service	Dr Ken Rice	1,500,000	1,098,949	401,051
y09	Director's Time	Directors Time	Service	Prof Arthur S Trew	29,685,133	82,538	764,170
<b>External Projects</b>							
t01	NIMES: New Improved Muds from Environmental Sources.	External	Class1a	Dr Chris Greenwell	4,113,669	4,245,424	-131,755
x01	HPC-Europa	External	Class1a	Dr Judy Hardy	16,415,790	8,925,197	7,490,593
x05	FIOS	External	Class1a	Mr Davy Virdee	1,130,100	1,074,930	55,170
e168	TEXT	External	Service	Dr Mark Bull	1,500,000	0	1,500,000
x02	BlueArc (TDS)	External	Service	Mr M W Brown	1,000	0	1,000
x06	Rhymney	External	Service	Dr Mark Sawyer	4,500	16	4,484