HECToR Quarterly Report

April - June 2010

1 Introduction

This report covers the period from 1 April 2010 at 0800 to 1 July 2010 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/2Q10.php

2 Executive Summary

- XT4 utilisation in 2Q10 was 75.3%, compared to 72.0% in 1Q10. Further details are available in Section 3.2 of the report.

- Low Priority Access accounted for 4.3% of the overall utilisation in 2Q10 and this initiative is expected to continue.

- As a result of the EPSRC Resource Allocation Panel (RAP) which was held in June, five Class 1b projects started on HECToR in June. A total of 12,436,320 AUs were allocated. Details of the Class 1b projects are included in Section 3.2.6.

- There were 16 service failures in 2Q10 as opposed to 14 in 1Q10. All 16 failures were attributed to technology problems. April was a particularly challenging month, with 10 service failures in total. The issues encountered during April were escalated to the highest level and were reviewed in detail by both the HECToR Scientific Advisory Committee (SAC) and Strategic Management Board (SMB). The overall MTBF decreased from 2Q10 from 157 to 137 hours.

- The volume of single node failures has remained constant from the previous quarter. There were 69 node failures in 2Q10, as opposed to 68 in 1Q10.

- The X2 vector system was very reliable in 2Q10. Charging remained suspended on the X2, resulting in an overall utilisation of 39.9%, compared to 56.9% in 1Q10. Further details on X2 utilisation are available in Section 3.2.2.

- At the Helpdesk, 1000 queries were resolved, compared to 1249 in 1Q10. User feedback was again varied in 2Q10, with a number of both positive and negative quality tokens received. An analysis of user quality tokens is contained in Section 4.1.

- 2Q10 was a very busy period as a result of the Phase 2b upgrade. The effort expended in May and June greatly exceeded the contractual service requirements.

- In 2Q10, the first phase of the Phase 2b upgrade took place. This included an operating system upgrade to CLE2.2, and the installation of the XT6. Both upgrades went very well. The Phase 2b system was made available to users on 10th June, and availability trials were completed on June 24th. Details of the upgrades are included in Section 5.1.

- Utilisation on the Phase 2b service between 10th and 28th June was 69%. This has since dropped and utilization to date in July is 20%. It is becoming clear that allocations do not match the increased capacity of the service. More details on this are available in Section 3.2.7

- The planned installation of the external Lustre filesystem in 2Q10 did not go ahead as planned. A number of issues were encountered in the early phases of the upgrade. This has now been postponed until 3Q10. Details are available in Section 5.1.4.

3 Quantitative Metrics

3.1 Reliability

The metrics in Section 3.1 relate solely to the service machine – i.e. the Cray XT4 (Phase 2a).

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

	April	*May*	*June*
Incidents	18	29	31
Failures	10	5	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*	*April*	*May*	*June*	*Quarterly*
Technology	Failures	10	5	1	16
	MTBF	73	146	732	137
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	10	5	1	16
	MTBF	73	146	732	137

3.2 HECToR Utilisation

3.2.1 XT4 Utilisation
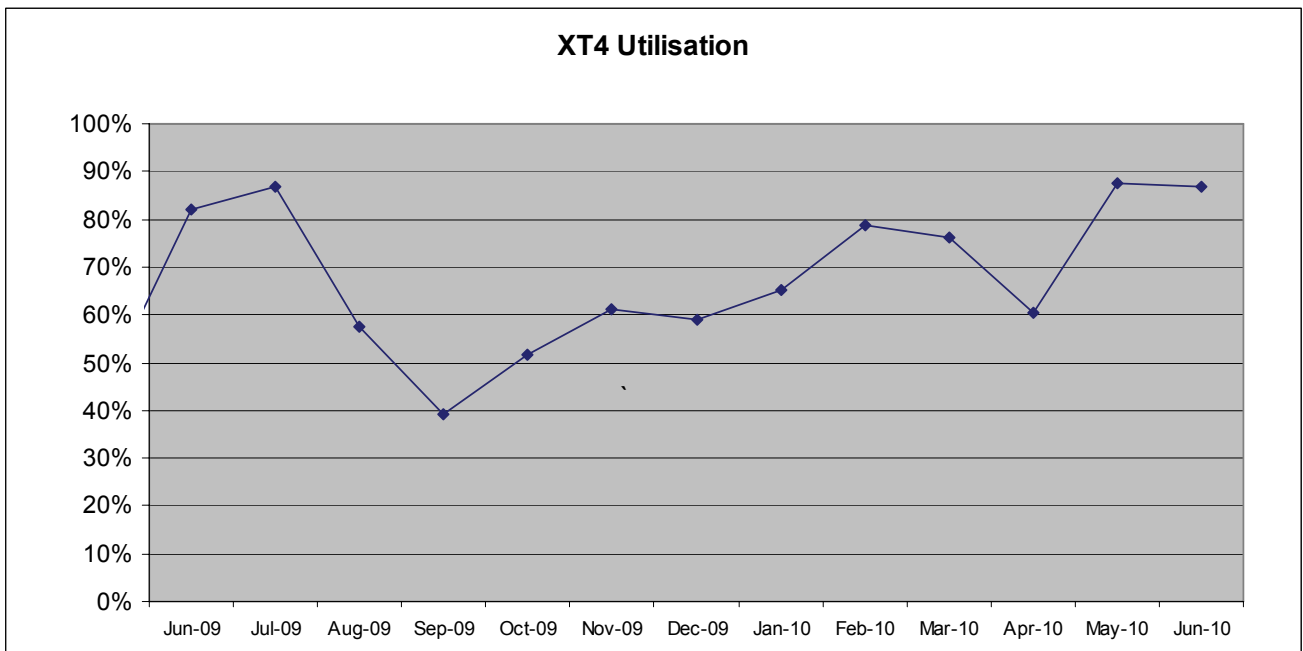
The XT4 utilisation quarterly average in 2Q10 was 75.3%, compared to 72% in 1Q10. Utilisation dropped in April as a result of reduced service availability although the system was very busy when it was available.
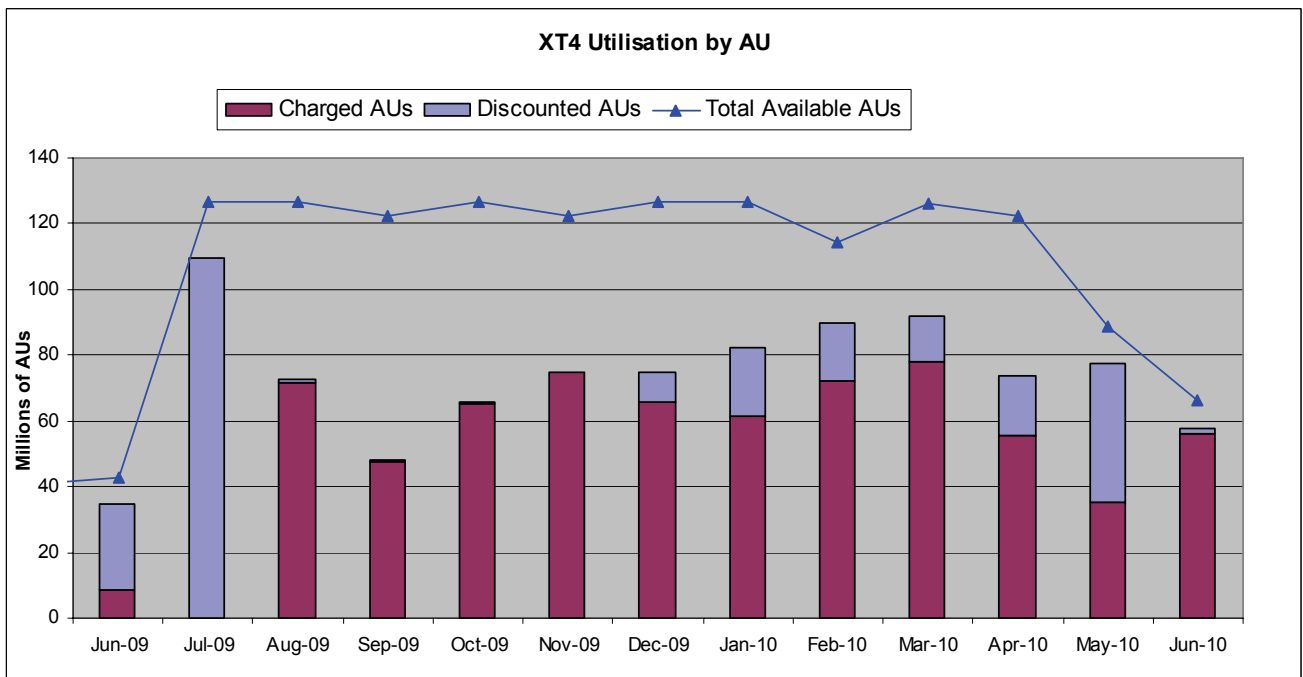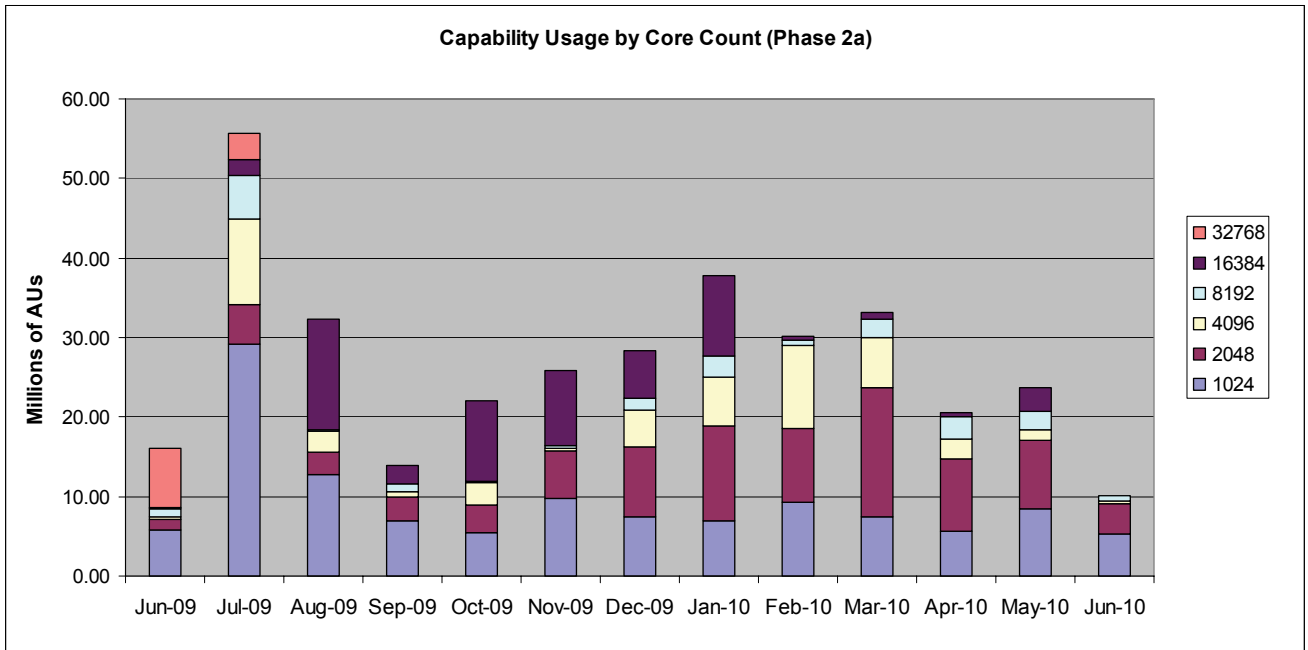

Charging was suspended on the XT4 from 27th April to 14th May hence the rise in discounted AUs. The XT4 was reduced in capacity from 60 to 33 cabinets on 12th May.

Capability Incentives

Capability usage was impacted in April due to the service issues. As of 12th May the largest job supported on the Phase 2a service is 8192 nodes

Capability incentives have been approved for the Phase 2b service and have been enabled as of 1st July. Capability incentives on Phase 2b will be reported as of 3Q10.

Low Priority Access

In 2Q10, low priority access accounted for 4.3% of the overall utilisation. During May and June, the service was so busy that only a few low priority jobs ran. This clearly illustrates that the initiative is working as intended. Low priority access is enabled also on Phase 2b.
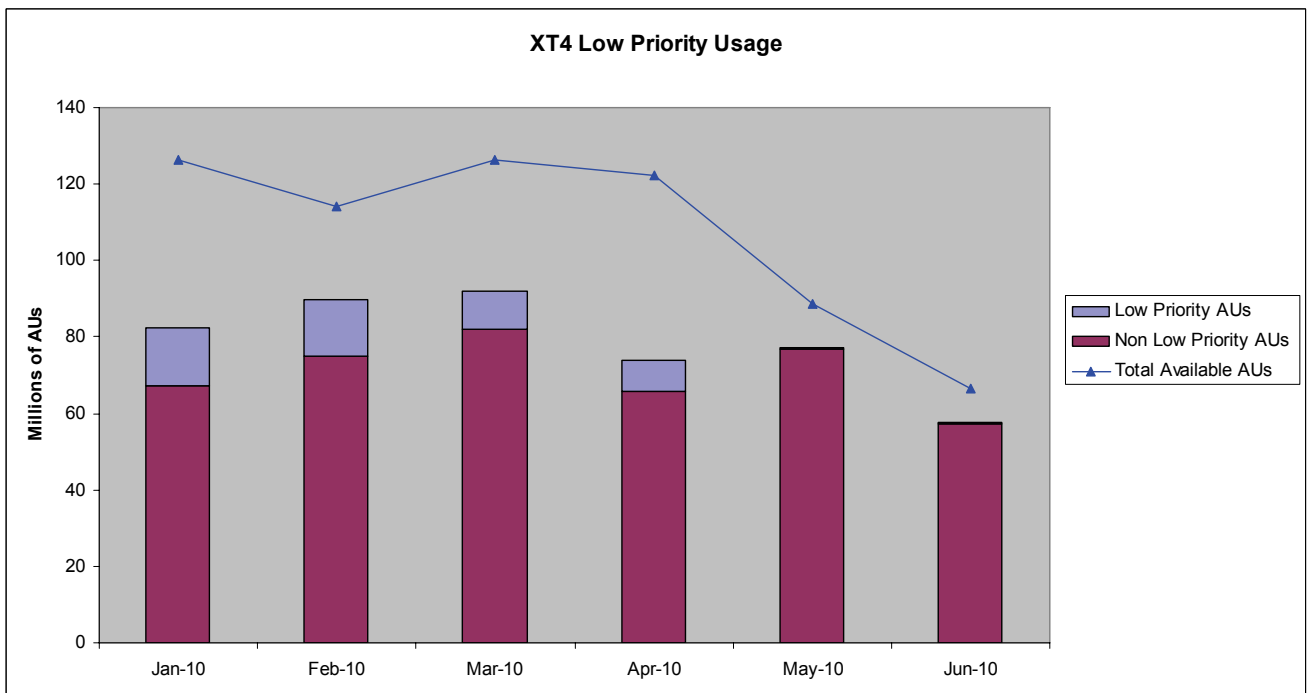
3.2.2 XT4 Utilisation by Core Count
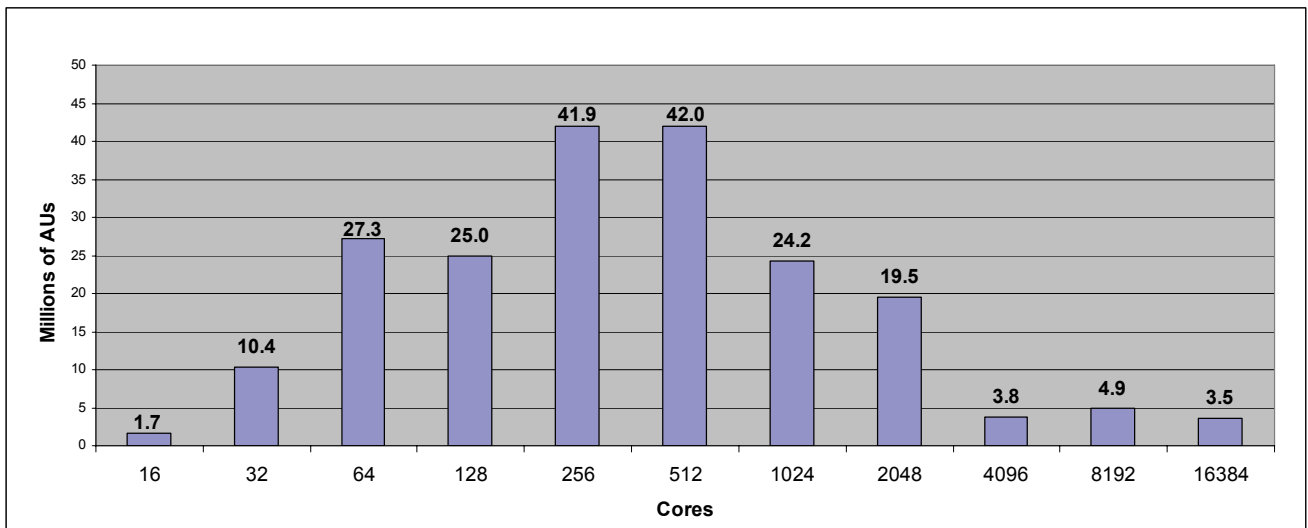
3.2.3 XT4 Number of Jobs by Core Count
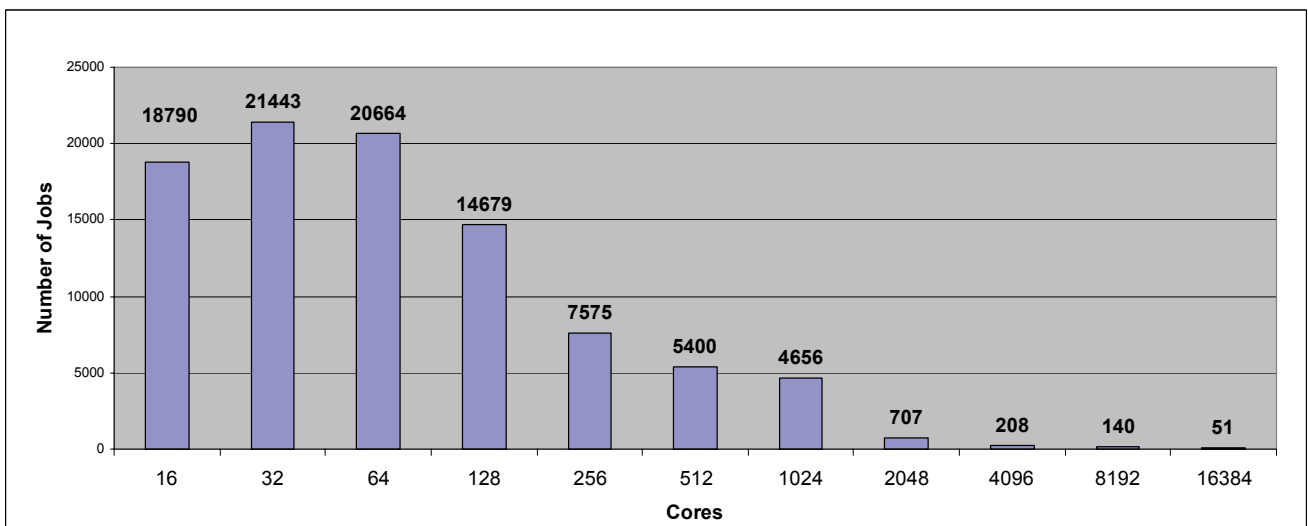
3.2.5 X2 Utilisation

Accounting remained suspended on the X2 throughout 2Q10. The peak in usage in February came primarily from the DEISA community
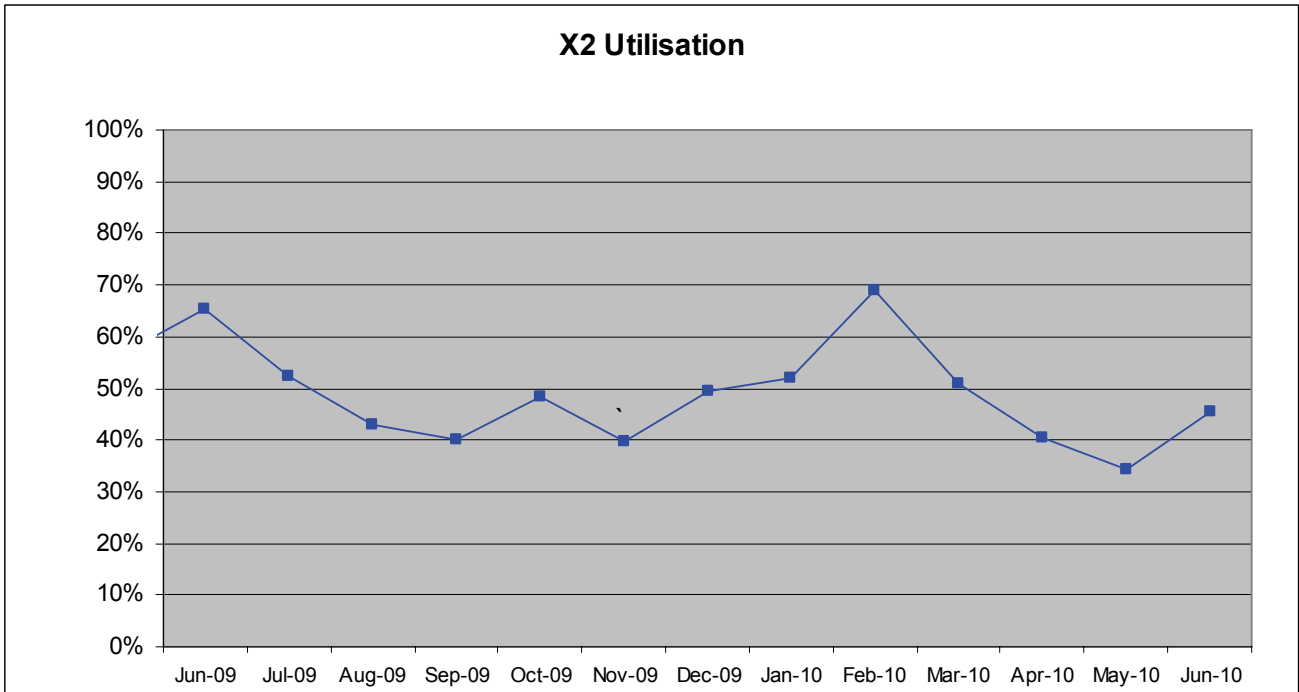
X2 Utilisation

The overall X2 utilisation for 2Q10 was 40%.

3.2.6 XT6 Utilisation

Early access users were granted access to the Phase 2b service on 10th June, and the remaining users were given access on 14th June.

Charging was initially suspended during the availability trial phase of the upgrade. The trial completed successfully on 24th June, and charging was enabled on 28th June. EPSRC and HSAC agreed that the Linpack-based AU rate should be discounted by 20% in order to allow for any performance impact whilst we await the Gemini interconnect. This discount can be adjusted flexibly to ensure good utilisation of both systems.

Between 10th and 28th June, utilisation on the Phase 2b service was 69%. This dropped very quickly when the charging was implemented. Utilisation for the month to date (as at 14th July) is only 20%. This clearly shows that users are inhibited by the notional cost of the service. As detailed below in Section 3.2.7, it is also becoming clear that the current AU allocations do not reflect the expanded size of the service.

3.2.4 Utilisation by Consortium

Project	XT4 Utilisation	XT6 Utilisation	X2 Utilisation
y02	2.40%	0.14%	0.00%
y03	0.00%	0.00%	0.00%
y04	0.00%	0.00%	0.00%
y05	0.01%	0.00%	0.00%
y06	0.00%	0.00%	0.00%
y07	0.00%	0.00%	0.00%
y11	0.00%	0.00%	0.00%
z01	0.11%	0.09%	0.00%
z02	0.02%	0.04%	0.00%
z03	0.23%	0.51%	0.00%
Internal Total	**2.76%**	**0.77%**	**0.00%**
c01	2.01%	0.15%	0.00%
e01	3.44%	0.30%	30.46%
e05	6.91%	2.72%	8.82%
e10	0.04%	0.00%	0.00%
e24	5.61%	0.58%	0.00%
e35	0.46%	0.00%	0.00%
e42	0.74%	0.00%	0.00%
e63	1.63%	0.79%	0.00%
e68	3.22%	9.34%	0.00%
e70	0.42%	0.88%	0.00%
e71	0.00%	0.00%	0.00%
e76	0.62%	0.00%	0.00%
e84	0.01%	0.00%	0.00%
e85	0.80%	1.42%	0.00%
e89	7.68%	22.77%	0.00%
e90	0.00%	0.00%	0.00%
e92	0.03%	0.17%	0.00%
e101	0.00%	0.00%	0.00%
e102	0.08%	0.00%	0.00%
e104	0.00%	0.00%	0.00%
e107	0.22%	0.00%	0.00%
e110	3.08%	0.83%	0.00%
e113	0.01%	0.00%	0.00%
e117	2.12%	0.00%	0.00%
e120	0.02%	0.00%	0.00%
e121	0.82%	0.00%	0.00%
e122	1.82%	1.66%	0.00%
e124	0.51%	0.56%	0.00%
e125	1.24%	0.33%	0.00%
e126	0.74%	0.00%	0.00%
e131	0.03%	0.00%	0.00%
e132	0.00%	0.00%	0.00%
e135	0.00%	0.00%	0.00%
e136	0.06%	0.00%	0.00%
e138	0.00%	0.00%	0.00%
e139	0.09%	0.00%	0.00%
e141	0.00%	0.00%	0.00%
e145	0.04%	0.00%	0.00%

Project	XT4 Utilisation	XT6 Utilisation	X2 Utilisation
e147	0.01%	0.00%	0.00%
e148	0.05%	0.56%	0.00%
e150	0.08%	0.00%	0.00%
e151	0.04%	0.00%	0.00%
e152	0.01%	2.32%	0.00%
e153	0.51%	0.09%	0.00%
e154	0.04%	0.00%	0.00%
e163	0.00%	0.00%	0.00%
e167	0.01%	0.00%	0.00%
e169	0.02%	0.00%	0.00%
EPSRC Total	**45.28%**	**45.54%**	**39.87%**
n01	3.79%	0.66%	0.00%
n02	10.59%	2.62%	0.00%
n03	7.71%	1.82%	0.00%
n04	2.11%	1.98%	0.00%
NERC Total	**24.21%**	**7.09%**	**0.00%**
b10	0.00%	0.00%	0.00%
b100	0.14%	0.00%	0.00%
BBSRC Total	**0.14%**	**0.00%**	**0.00%**
p01	0.03%	0.00%	0.00%
STFC Total	**0.03%**	**0.00%**	**0.00%**
t01	0.29%	0.00%	0.00%
x01	2.31%	0.81%	0.00%
External Total	**2.65%**	**0.81%**	**0.00%**
d03	0.06%	0.00%	0.00%
d04	0.00%	0.04%	0.01%
d11	0.00%	0.00%	0.00%
d14	0.02%	11.19%	0.00%
d15	0.00%	0.00%	0.00%
d18	0.00%	0.03%	0.00%
d19	0.15%	0.00%	0.00%
d21	0.01%	0.00%	0.00%
d22	0.01%	0.00%	0.00%
DirectorsTime Total	**0.25%**	**11.27%**	**0.07%**
Total	**75.32%**	**65.48%**	**39.94%**

Note – the figures here for the XT6 are from 10th June only.

3.2.6 Direct Access Projects

Six direct access (Class 1b) projects started on HECToR in March. These direct access projects are approved on a 'use it or lose it' basis. They have a fixed timescale after which any unused AUs will be lost.

Project	Principle Investigator	Start Date	End Date	AUs Allocated	Discounted AUs Used	Charged AUs Used
e125	Alivi	30/03/2010	30/09/2010	3,072,000	1,530,958	1,897,378
e150	Ballone	01/03/2010	01/10/2010	1,800,000	0	214,399
e151	Ganapathisubramani	01/03/2010	01/10/2010	1,270,000	0	122,695
e152	Vanreeuwijk	01/03/2010	01/10/2010	7,500,000	2	35,675
e153	Tilocca	01/03/2010	01/10/2010	2,000,000	218,228	1,187,154
e154	Morrison	01/03/2010	01/10/2010	2,000,000	0	115,470
e117	Domene	07/03/2010	07/10/2010	12,000,000	2,558,514	3,329,532

The direct access projects which started in March accounted for 3.2% of the utilisation on the service in 2Q10. Based on the allocations and the fixed project durations, we would have expected the usage from these projects in 2Q10 to have been higher.

An additional 5 projects were approved in June.

Project	Principle Investigator	Start Date	End Date	AUs Allocated
e170	Morgan	01/07/2010	01/10/2010	1,935,360
e136	Harrison	28/06/2010	28/12/2010	5,300,000
e82	Dawes	28/06/2010	28/12/2010	2,496,000
e82	Haynes	01/07/2010	01/01/2011	1,000,000
e171	Persson	12/07/2010	12/01/2011	1,704,960

3.2.7 HECToR Usage Forecast

The graph below shows the available capacity of the service in AU/Hour, versus the actual allocation of AUs to projects. The available capacity is represented by the two lines (at 100% and 80%).
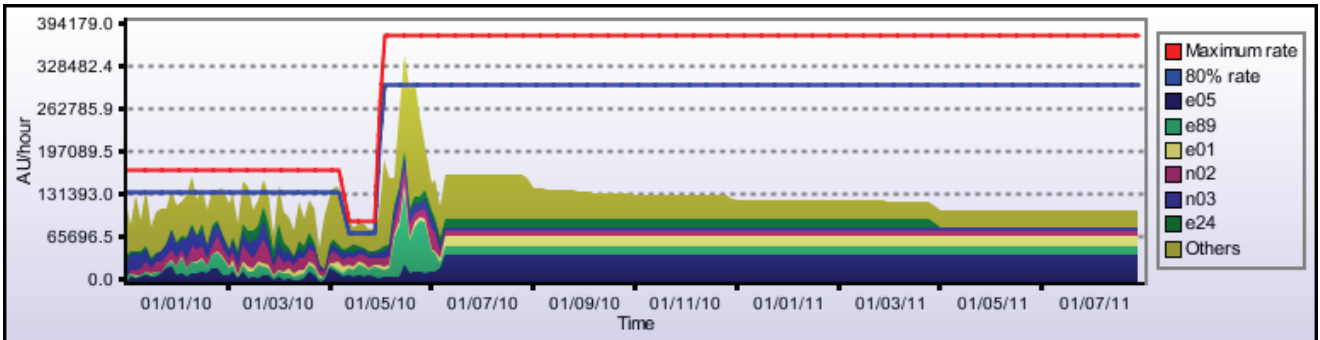
For historic data, the project data shown reflects actual AU usage. The future view is based on the forecast usage profile per project. This is determined by the total AUs allocated and the project end-date. This provides a flat forecast profile month-on-month per project. There is the facility within SAFE for PIs to set more accurate profiles, but this does not get used.

It is clear from the above graph that since the growth in capacity with the arrival of the Phase 2b system, that the HECToR service is significantly under-allocated.

3.3. Performance Metrics

All performance metrics relate solely to the service machine – i.e. the Cray XT4 (Phase 2a).

Metric	TSL(%)	FSL(%)	Apr-10	May-10	Jun-10	2Q10
Technology reliability (%)	85.00%	98.50%	80.9%	98.6%	99.3%	93.0%
Technology MTBF (hours)	100	126.4	73.3	146.4	732.0	137.3
Technology Throughput, hours/year	7000	8367	6984	8393	8636	8004
Capability jobs completion rate	70%	90%	97.4%	94.3%	100.0%	97.2%
Non in-depth queries resolved within 1 day (%)	85%	97%	98.7%	98.2%	98.7%	98.5%
Number of SP FTEs	7.3	8.0	8.6	10.3	10.7	9.9
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

4. Helpdesk

A total of 1000 queries with a specified service metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	847	860	98.5%	97.0%
Admin queries finished in 1 day	755	762	99.1%	97.0%
Queries assigned in 30 min	989	991	99.8%	97.0%
Technical assessments in 10 days	25	26	96.2%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	537	53.7%
Admin	225	22.5%
In-depth	114	11.4%
Technical	98	9.8%
Technical assessment class-1	21	2.1%
Technical assessment class-2	5	0.5%

Queries by Category

Query Category	Queries	Percentage
Set group quotas	198	19.8%
Set user quotas	105	10.5%
New User	98	9.8%
New Password	70	7.0%
Access to HECToR	70	7.0%
3rd Party Software	47	4.7%
Node Failure	46	4.6%
Disk, tapes, resources	45	4.5%
User behaviour	43	4.3%
Batch system and queues	36	3.6%
None	30	3.0%
Compilers and system software	25	2.5%
Join Project	22	2.2%
Archive	22	2.2%
Login, passwords and ssh	19	1.9%
New Group	17	1.7%
User programs	16	1.6%
Performance and scaling	14	1.4%
Other	14	1.4%
Add to group	14	1.4%
SAFE	13	1.3%
Create certificate	7	0.7%
Update account	6	0.6%

Static website	6	0.6%
Remove account	6	0.6%
Grid	4	0.4%
Courses	4	0.4%
Porting	1	0.1%
Delete from group	1	0.1%
Delete Certificate	1	0.1%

Queries by Handler Category

Handlers	Total	Automatic	Admin	In-depth	Technical	Technical assessment class-1	Technical assessment class-2	%age
OSG	599	537	13	14	35			59.9%
USL	298		211	38	49			29.8%
CSE	64			38		21	5	6.4%
Cray Systems	39		1	24	14			3.9%

4. 1 Quality Tokens

A number of quality tokens were set by users during 2Q10.

Project	Negative Tokens	Positive Tokens
e05	5	0
n02	16	0
x01	0	5
Total	**21**	**5**

The negative quality tokens were related to system unavailability, queuing time during the discounted period in May and one delayed query. n02 users were clearly unhappy.

5 System Hardware

5.1 HECToR Technology Changes

5.1.1 Operating System Upgrade

The HECToR operating system was upgraded to CLE2.2 in April. There were no major issues encountered. The lessons learned during the previous upgrade from CLE2.0 to CLE2.1 were clearly beneficial in ensuring that the process went smoothly.

5.1.2 Phase 2a Capacity Reduction

As part of the Phase 2b upgrade process, the XT4 system was reduced in capacity from 60 to 33 cabinets. This took place on 19th May as planned. No issues were encountered with the change.

5.1.3 Phase 2b Installation

The Phase 2b upgrade ran very smoothly. The hardware was delivered and installed as planned, and acceptance tests were completed in early June. Early access users were granted access to the service on 10th June, and the remaining users were given access on 14th June.

5.1.4 esFS Upgrade

A migration to external Lustre (esFS) was originally planned for 2Q10. Due to the major issues encountered in April which were discussed at both HSAC and SMB, this has now been delayed until later in 3Q10. The Phase 2b system went live with its own directly attached filesystem as a result. The exact dates for the esFS upgrade are currently unclear but will be published as soon as they are available.

5.2 Severity-1 Incidents

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

	April	*May*	*June*
Incidents	18	29	31
Failures	10	5	1

Technology failures were responsible for 12 of the Severity-1 incidents during 2Q10. Of the12 technology failures, 4 related to Lustre and external Lustre. In addition, there were 2 maintenance overruns, and 2 errors as a result of operator error. There were no Service Provision failures in 2Q10.

5.3 Single Node Failures

There were 69 node failures in 2Q10 compared to 68 in 1Q10. Only 7 of these were related to specific hardware faults (Dimm failures/Opteron cache errors). Looking at the trends in the different types of error, it can be seen from the graph below that the number of communications errors trends closely to utilisation.

Comms Fails V Utilisation
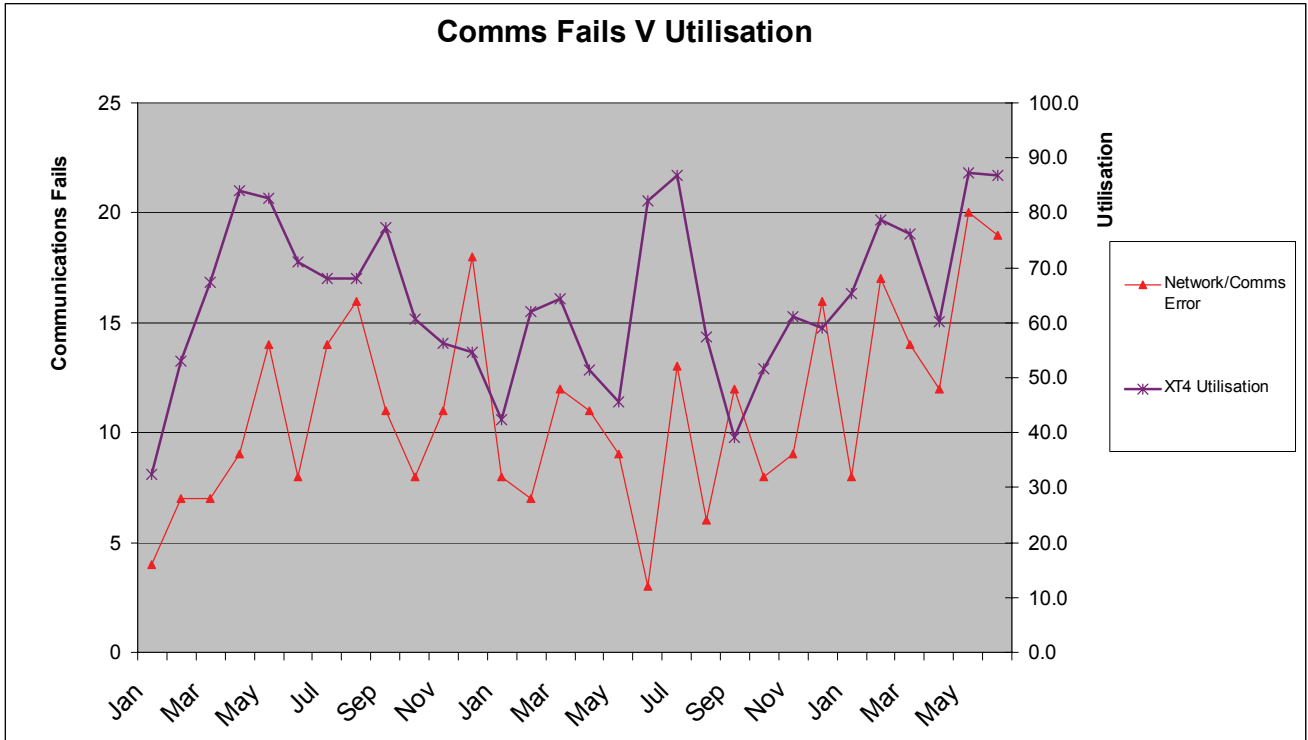
Appendix A: Terminology

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	Title	Funding Body	Class	PI	Total AUs Allocated	AUs used	AUs left
EPSRC							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Richard Blake	30,803,723	22,006,510	8,797,213
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969,876	13,807,693	470,162,183
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124,000	80,277,956	1,058,786,044
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	10,248,188	6,168,577	4,079,611
e24	DEISA	EPSRC	Class1a	Mrs Alison Kennedy	168,707,436	78,734,435	89,973,001
e35	Non-adiabatic processes	EPSRC	Class1a	Dr Tchavdar Todorov	12,246,862	4,158,494	8,088,368
e59	Turbulence in Breaking Gravity Waves	EPSRC	Class1a	Prof Ian P Castro	708,922	440,752	268,170
e63	UK Applied Aerodynamics Consortium 2	EPSRC	Class1a	Dr Nick Hills	30,925,323	16,603,898	14,321,425
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000,000	38,594,401	11,405,599
e70	Computation of Electron Transfer Properties	EPSRC	Class1a	Dr Jochen Blumberger	1,160,000	1,154,375	5,625
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403,522	40,203,133	90,200,389
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521,798	27,862,753	14,659,045
e77	Porting of DFT/GW Codes	EPSRC	Class2a	Prof Maria Merlyne DeSouza	160,000	60,676	99,324
e81	e-Collision experiments using HPC	EPSRC	Class2a	Prof NS Scott	257,095	25,697	231,398

Code	Title	Funding Body	Class	PI	Total AUs Allocated	AUs used	AUs left
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	1,105,352	101,352	1,004,000
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600,000	99,364	9,500,636
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	5,588,610	2,072,143	3,516,467
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	360,000,001	128,043,736	231,956,265
e90	Network modelling of wireless cities	EPSRC	Class2a	Prof Jonathan M Pitts	100,000	58,608	41,392
e92	Dynamo Action In Compressible Convection	EPSRC	Class1a	Mr Paul Bushby	4,075,000	451,556	3,623,444
e101	Optimization of HPCx LES code	EPSRC	Class2a	Prof Michael Leschziner	641,009	642,368	-1,359
e102	Numerical investigation of aerofoil noise	EPSRC	Class1a	Dr Richard D Sandberg	6,484,191	5,962,738	521,453
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	2,400,000	66,224	2,333,776
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	158,044	5,841,956
e108	Unsteady Propeller Noise	EPSRC	Class2b	Dr Sergey Karabasov	415,632	158,100	257,532
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	39,100,000	18,054,833	21,045,167
e113	[dCSE] MRBV ? Massive Remove Batch Visualizer	EPSRC	Class2b	Dr Martin Turner	85,440	45,301	40,139
e115	Multiscale Modelling of Biological Systems	EPSRC	Class2a	Prof Jonathan W Essex	100,000	0	100,000

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e117	Binding free energy estimations	EPSRC	Class1b	Dr Carmen Domene	12,247,664	3,735,667	8,511,997
e119	Nanoscale Energy Transportation	EPSRC	Class2a	Dr Dongsheng Wen	100,000	0	100,000
e120	[dCSE] FF Transformations for plasma simulations	EPSRC	Class2b	Dr Colin M Roach	200,000	124,875	75,125
e121	[dCSE] Improving Performance using Wannier functions	EPSRC	Class1a	Prof Maria Merlyne DeSouza	2,680,305	1,469,569	1,210,736
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	65,000,000	15,879,228	49,120,772
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Dr Richard D Sandberg	22,887,943	5,617,432	17,270,511
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1b	Dr Ali Alavi	3,324,825	3,051,783	273,042
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	9,984,000	2,685,844	7,298,156
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000,000	144	6,999,856
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	0	7,500,000
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	200,000	70,106	129,894
e132	Parallel Version of a Design Sensitivity Tensegrity Code	EPSRC	Class2a	Prof Rod Smallwood	200,000	18,431	181,569
e133	Implementation of Established Algorithms to Extend HELIUM	EPSRC	Class2b	Prof Ken Taylor	400,000	0	400,000
e134	Numerical Simulation of Turbomachinery Flows	EPSRC	Class2a	Dr Francesco Montomoli	200,000	16,419	183,581

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e135	DNS of unsteady turbulent flow over a smooth or a rough surface	EPSRC	Class2a	Dr Shuisheng He	200,000	91,361	108,639
e136	Modelling the UK Wind Power Resource	EPSRC	Class1b	Dr Gareth Harrison	5,679,268	284,492	5,394,776
e137	Turbulent Pipe Flow	EPSRC	Class2a	Prof Dwight Barkley	200,000	199,832	168
e138	[dCSE] Naturally occurring magnetic mineral systems on HECToR	EPSRC	Class2b	Prof Wyn Williams	400,000	180	399,820
e139	Scalability Optimization for Largescale in-silico Simulations	EPSRC	Class2b	Dr Gernot Plank	400,000	421,138	-21,138
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350,000	12,758	16,337,242
e142	A Study of Doped Semiconducting Nanowires	EPSRC	Class2a	Mr Arash A Mostofi	200,000	198,094	1,906
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	85,056	1,106,843
e146	G protein-coupled receptor dynamics	EPSRC	Class2a	Dr Irina Tikhonova	199,680	0	199,680
e147	Scale adaptive simulations of turbulent flows	EPSRC	Class2a	Prof Oubay Hassan	200,000	109,710	90,290
e148	Adding the molecular dynamics functionality to the quantum	EPSRC	Class2b	Prof Dario Alfe`	400,000	156,411	243,589
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	51,920,000	0	51,920,000
e150	Actin and tubulin polymerisation	EPSRC	Class1b	Dr Pietro Ballone	1,800,000	314,313	1,485,687
e151	Fine-scale turbulence in mixing layers	EPSRC	Class1b	Dr Bharathram Ganapathisubramani	1,270,000	323,265	946,735
e152	Turbulent entrainment	EPSRC	Class1b	Dr Maarten van Reeuwijk	7,500,000	43,217	7,456,783

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e153	Maya Blue Hybrid Materials	EPSRC	Class1b	Dr Antonio Tilocca	2,000,000	1,838,696	161,304
e154	Fast proton transport in biological systems	EPSRC	Class1b	Dr Carole A Morrison	2,000,000	115,420	1,884,580
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	400,000	0	400,000
e157	Global stability computations of separated flows	EPSRC	Class2a	Prof Jitesh S B Gajjar	200,000	8	199,992
e162	Study of Energetic Materials	EPSRC	Class2a	Dr Carole A Morrison	201,600	0	201,600
e163	Numerical Simulation of Spontaneous Ignition	EPSRC	Class2a	Prof Jennifer Wen	200,000	184	199,816
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	200,000	0	200,000
e167	LES of supersonic jets	EPSRC	Class1b	Prof William Dawes	2,696,000	19,254	2,676,746
e168	TEXT	External	Service	Dr Mark Bull	1,500,000	0	1,500,000
e169	Oxygen reduction reaction on platinum nanoalloys	EPSRC	Class2a	Dr Francesca Baletto	200,000	213,544	-13,544
e170	CFD Simulations of the BLOODHOUND SuperSonic Car	EPSRC	Class1b	Dr Ken Morgan	1,935,360	0	1,935,360
e171	Conformational switching of tetra-(bromophenyl) porphyrins	EPSRC	Class1b	Prof Mats Persson	1,704,960	0	1,704,960
e172	HPC environment for realistic cardiac simulations	EPSRC	Class2a	Dr Irina V. Biktasheva	200,000	0	200,000
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class2a	Prof Matthias Heil	200,000	0	200,000

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NERC							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Thomas Anderson	89,243,840	36,160,222	53,083,618
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Lois Steenman-Clark	258,768,327	144,648,628	114,119,699
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	284,142,416	185,496,448	98,645,968
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	112,202,935	52,492,127	59,710,808
BBSRC							
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	549,363	1,450,637
b10	SPRINTing with HECToR [dCSE]	BBSRC	Class2b	Mr Terry Sloan	400,000	4,880	395,120
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10,000,000	373,476	9,626,524
b11	ExeterBioSeq	BBSRC	Class2a	Prof Richard ffrench-Constant	200,000	0	200,000
STFC							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	3,020,000	75,502	2,944,498
External							
t01	NIMES: New Improved Muds from Environmental Sources.	External	Class1a	Dr Chris Greenwell	4,113,669	3,166,674	946,995
x01	HPC-Europa	External	Class1a	Dr Judy Hardy	8,566,434	5,391,809	3,174,625

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Directors Time							
d03	EUFORIA	DirectorsTime	Service	Mr Adrian Jackson	2,200,000	1,288,286	911,714
d04	MSc in HPC	DirectorsTime	Service	Dr David Henty	343,500	75,174	268,326
d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	416,667	37,001	379,666
d12	CoE HiGEM	DirectorsTime	Service	Dr Len L C Shaffrey	10,000,000	0	10,000,000
d13	CoE SENGA	DirectorsTime	Service	Dr Stewart Cant	10,000,000	0	10,000,000
d14	CoE HiPSTAR	DirectorsTime	Service	Dr Richard D Sandberg	2,000,000	2,264,689	-264,689
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	2,033	1,037	996
d16	ETC	DirectorsTime	Service	Dr Lorna Smith	501,000	8,850	492,150
d18	FireGrid HPC	DirectorsTime	Service	Prof Arthur S Trew	600,001	52,562	547,439
d19	OpenFOAM Demo	DirectorsTime	Service	Dr Alan Gray	950,000	385,565	564,435
d20	CSCS	DirectorsTime	Service	Dr Alan Gray	50,000	0	50,000
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1,000,001	18,584	981,417
d22	Summer Science Exhibition	DirectorsTime	Service	Prof. Angelos Michaelides	70,000	35,572	34,428
d23	TEXT FP7	DirectorsTime	Service	Dr Mark Bull	1,500,000	3,761	1,496,239