HECToR Quarterly Report

April - June 2009

1 Introduction

This report covers the period from 1 April 2009 at 0800 to 1 July 2009 at 0800.

Section 3 summarises service availability, performance statistics and utilisation for this quarter. Section 4 shows Helpdesk statistics. An overview of system hardware changes, service failures, and node failures is available in Section 5. A summary table of the key performance metrics is given in the final section.

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/2Q09.php

2 Executive Summary

- 2Q09 has been the key transitional period the service has been through to date, with both the operating system upgrade to CLE2.1 and the compute node upgrade to quad-core nodes taking place during this timeframe.

- The HECToR operating system was upgraded to CLE2.1 on 6th May. The upgrade which had been rescheduled from March was completed as planned. Major problems were subsequently identified regarding the Unified Model. A post–mortem was conducted by the service and key lessons were learned for future upgrades. Further details of the OS upgrade are available in Section 5.1.1.

- The HECToR Phase2a upgrade to quad-core was completed in June. Work commenced on the two-phase upgrade on 8th June and by June 29th HECToR was available to users with 5664 quad-core nodes. A test Linpack run demonstrated a maximum performance of 174 TFlops. This would have placed HECToR at theoretical sixteenth place in the June edition of the Top500. The acceptance testing and the availability trials will be run in July. More details of the work undertaken are available in Section 5.1.2.

- XT utilisation in 2Q09 was 60%. This was on a par with 1Q09 at 56%. User accounting was suspended on 19th June as part of the Phase2a upgrade process, resulting in 95% utilisation during the remainder of June. Further details are available in Section 3.2 of the report. Work is ongoing by both the service and EPSRC to review what can be done to improve utilisation on HECToR in the longer term.

- There were 8 service failures in Q209 which is a significant improvement on the 16 failures seen in 1Q09. All 8 failures were attributed to technology problems. Further details on the failures are available in Section 3.1. The overall MTBF increased on 1Q09 from 137 to 274 hours.

- The volume of single node failures has remained comparable to the previous quarter. There were 68 node failures in 2Q09, as opposed to 63 in 1Q09. We are continuing to track and investigate the cause of all failures and an analysis of these can be found in Section 5.3 of this report.

- The X2 Vector system was very reliable in 2Q09. Accounting remained suspended throughout 2Q09, resulting in an overall utilisation of 61%. Further details on the impact of the suspension of X2 accounting are available in Section 3.2.5.

- The helpdesk statistics were again excellent. Positive user feedback has been received with regard to the support teams, although there has been some negative feedback in relation to system reliability. The volume and type of queries received at the helpdesk remained constant from 1Q09.

- The HECToR website was updated in 2Q09 in parallel with the upgrade to quad-core nodes. The CSE and User Support teams worked well together to ensure there was a seamless transition of the web content. The source code branching method adopted for this upgrade will be reused for all future upgrades as this worked well. There is a

new look to the website along with changes to the HECToR technical specifications, user guide and frequently asked questions. The user support and liaison team are currently reviewing options for adding general HPC/HECToR ‘introductory’ views on the website, with a view to implementing these later in 2009.

3 Quantitative Metrics

3.1 Reliability

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

	April	*May*	*June*
Incidents	31	27	29
Failures	3	2	3

3.1.1 Performance Statistics

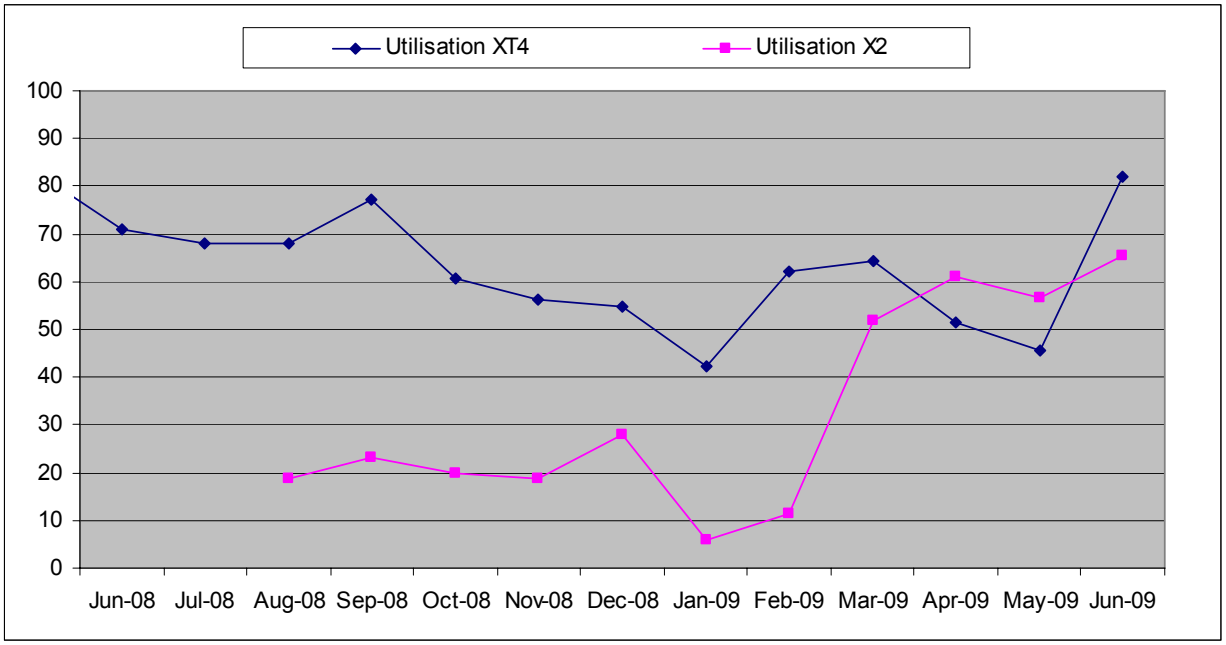
- MTBF = (732)/(number of failures in a month)

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

Attribution	*Metric*	*April*	*May*	*June*	*Quarterly*
Technology	Failures	3	2	3	8
	MTBF	244	366	244	274
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	3	2	3	8
	MTBF	244	366	244	274

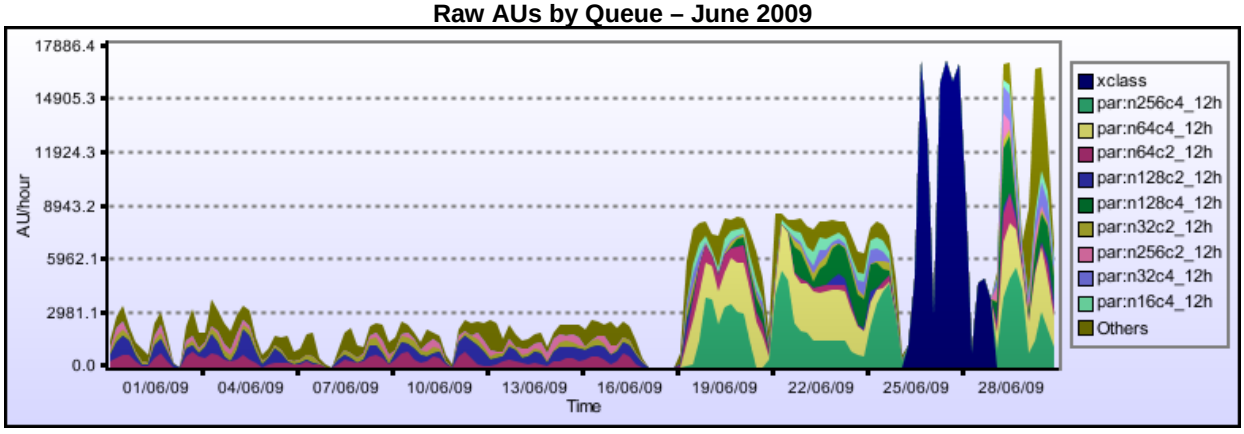
3.2 HECToR Utilisation

3.2.1 Overall Utilisation



Utilisation on the XT decreased slightly over the first two months of 2Q09. The peak in utilisation seen in June was as a result of the open access during the quad-core upgrade. Accounting was suspended on 19th June when HECToR became available at 50% quad-core. As of 29th June the service was available fully quad-core. As illustrated below users were quick to take advantage of the available resources. There was also minimal service downtime as a result of the upgrade. Note: The 'xclass' jobs which ran 26-29 June were the Linpack and Helium test jobs run by the Cray Centre of Excellence as part of the pre-acceptance testing phase.

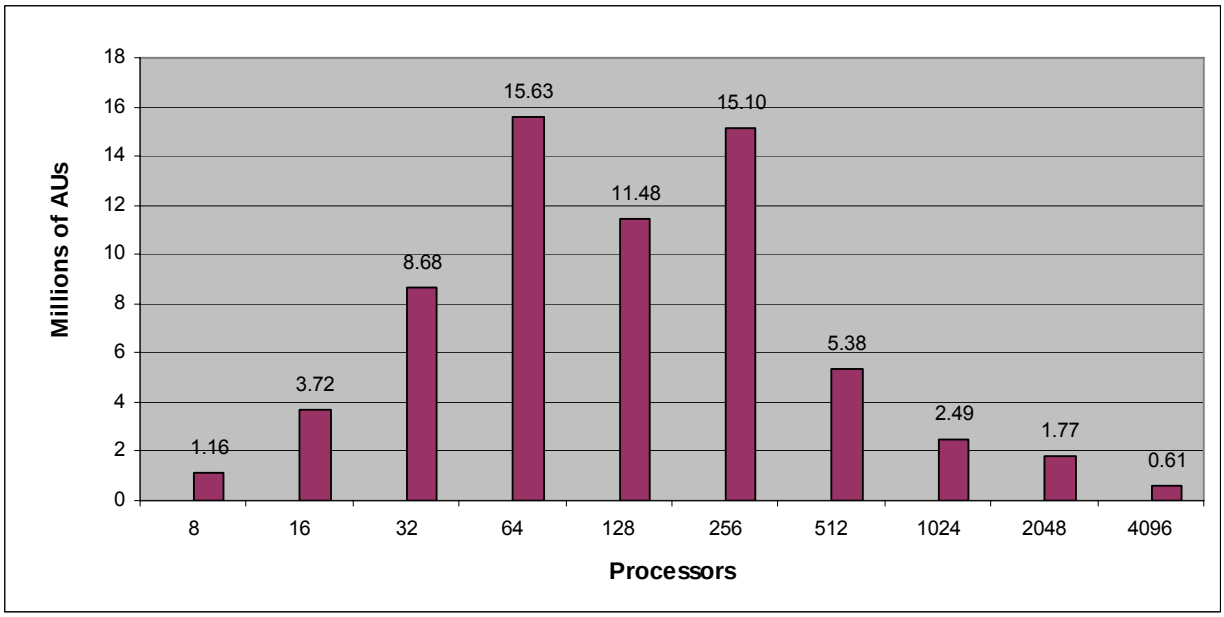
Raw AUs by Queue – June 2009



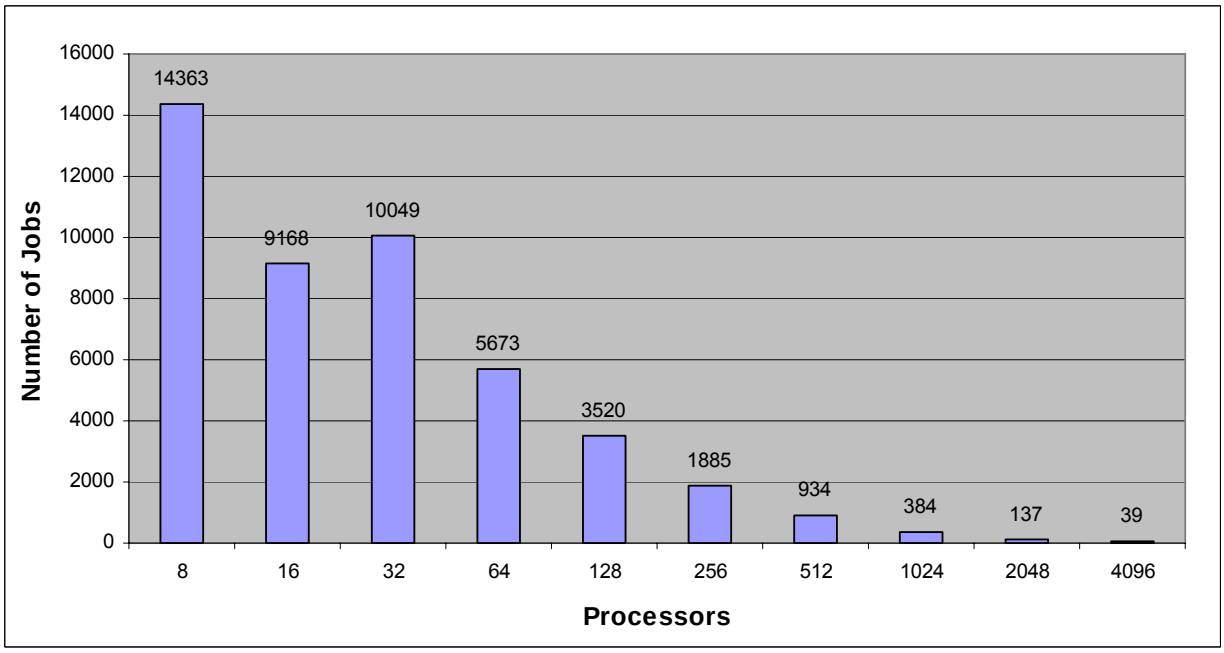
The service is currently reviewing options for increasing utilisation in the longer term. These include proposals for capability incentives for large jobs (similar to those on HPCx), discounted queues and revised compute resource allocation models.

The X2 open access initiative continued to have a marked effect on the utilisation of the X2. Details of this are available in Section 3.2.5.

3.2.2 XT Utilisation by Queue



3.2.3 XT Number of jobs per queue



3.2.4 Utilisation by Consortium

3.2.4.1 XT Utilisation by Consortium

Project	Raw AUs	Number of Jobs	Raw %age	Utilisation
y01	9,078	59	0.01%	0.01%
y02	88	4	0.00%	0.00%
y03	237	1078	0.00%	0.00%
y05	7,752,999	675	10.53%	6.33%*
y06	18	2115	0.00%	0.00%
y07	61	35	0.00%	0.00%
z01	377,651	1321	0.51%	0.31%
z02	3,257	468	0.00%	0.00%
z03	440,473	4618	0.60%	0.36%
z06	1,159	4	0.00%	0.00%
Internal Total	**8,585,021**	**10377**	**11.66%**	**7.01%**
c01	1,698,578	1946	2.31%	1.39%
e01	146,336	144	0.20%	0.12%
e05	3,837,805	2392	5.21%	3.13%
e100	1,543	9	0.00%	0.00%
e101	31,544	88	0.04%	0.03%
e102	839,173	307	1.14%	0.68%
e109	32,486	12	0.04%	0.03%
e110	1,127,319	354	1.53%	0.92%
e111	1,363	3	0.00%	0.00%
e113	3	24	0.00%	0.00%
e116	864	111	0.00%	0.00%
e119	0	7	0.00%	0.00%
e122	2,327,723	348	3.16%	1.90%
e125	4	16	0.00%	0.00%
e24	1,547,337	474	2.10%	1.26%
e35	150,637	143	0.20%	0.12%
e42	792,425	358	1.08%	0.65%
e63	2,358,087	765	3.20%	1.92%
e68	5,801,551	1924	7.88%	4.74%
e69	3,537	6	0.00%	0.00%
e70	82,418	203	0.11%	0.07%
e71	211,156	371	0.29%	0.17%
e72	7	9	0.00%	0.00%
e75	1,853,029	168	2.52%	1.51%
e76	444,363	31	0.60%	0.36%
e79	5	3	0.00%	0.00%
e81	5	15	0.00%	0.00%
e82	42	22	0.00%	0.00%
e84	5,574	125	0.01%	0.00%
e85	13,735	33	0.02%	0.01%
e89	14,064,937	5327	19.10%	11.48%
e90	36,900	394	0.05%	0.03%
e94	106,466	145	0.14%	0.09%
u03	11	7	0.00%	0.00%
u10	257,928	488	0.35%	0.21%
EPSRC Total	**37,774,891**	**16772**	**51.30%**	**30.83%**

*The high usage by y05 (Cray Centre of Excellence) was as a result of Linpack and Helium test runs.

Project	Raw AUs	Number of Jobs	Raw %age	Utilisation
n01	1,370,901	1866	1.86%	1.12%
n02	8,866,065	19671	12.04%	7.24%
n03	11,306,563	4456	15.35%	9.23%
n04	2,444,300	1527	3.32%	2.00%
NERC Total	**23,987,829**	**27520**	**32.58%**	**19.58%**
b01	298,658	29	0.41%	0.24%
b08	19,702	95	0.03%	0.02%
BBSRC Total	**318,360**	**124**	**0.43%**	**0.26%**
T01	92,938	129	0.13%	0.08%
x01	836,415	549	1.14%	0.68%
External Total	**929,352**	**678**	**1.26%**	**0.76%**
d03	1,256,141	462	1.71%	1.03%
d04	98,417	869	0.13%	0.08%
d07	217,973	68	0.30%	0.18%
d08	11,771	17	0.02%	0.01%
d09	457,040	190	0.62%	0.37%
DirectorsTime Total	**2,041,341**	**1606**	**2.77%**	**1.67%**
Total	**73,636,794**	**57077**	**100.00%**	**60.11%**

3.2.4.2 X2 Utilisation by Consortium

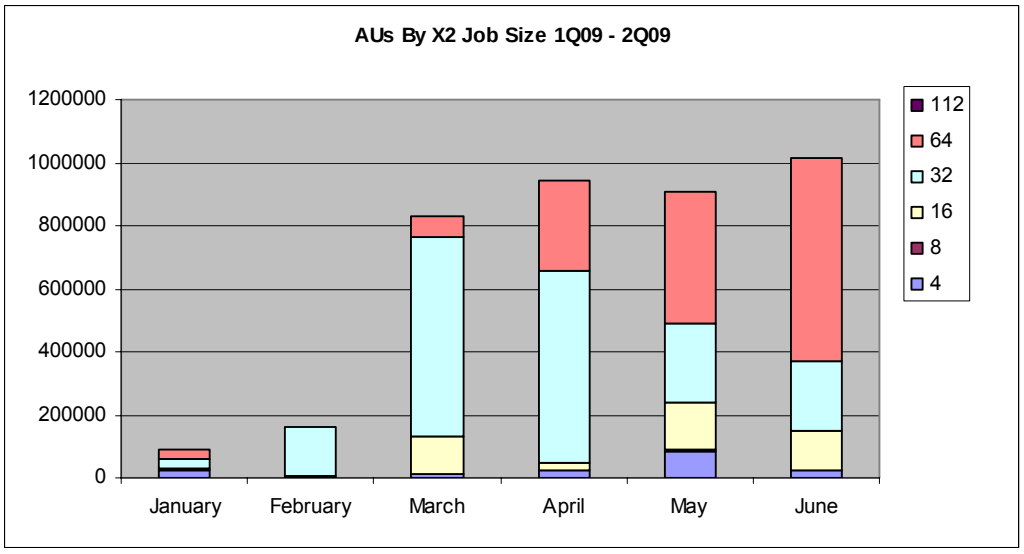
Project	Raw AUs	Number of Jobs	Raw %age	Utilisation
y02	129	20	0.00%	0.00%
y03	200	134	0.01%	0.00%
z01	307	3	0.01%	0.01%
z02	6	1	0.00%	0.00%
z03	984	100	0.03%	0.02%
Internal Total	**1,626**	**258**	**0.06%**	**0.03%**
e01	978,887	175	34.12%	20.84%
e05	1,083,309	391	37.76%	23.07%
e110	1	1	0.00%	0.00%
e123	1,421	17	0.05%	0.03%
e24	32,772	83	1.14%	0.70%
e69	1,274	12	0.04%	0.03%
e75	124,718	295	4.35%	2.66%
e85	51,980	58	1.81%	1.11%
e89	588,611	114	20.52%	12.53%
EPSRC Total	**2,862,972**	**1146**	**99.80%**	**60.96%**
n02	2,252	127	0.08%	0.05%
NERC Total	**2,252**	**127**	**0.08%**	**0.05%**
x01	1	1	0.00%	0.00%
External Total	**1**	**1**	**0.00%**	**0.00%**
d04	1,855	88	0.06%	0.04%
DirectorsTime Total	**1,855**	**88**	**0.06%**	**0.04%**
Total	**2,868,705**	**1620**	**100.00%**	**61.08%**

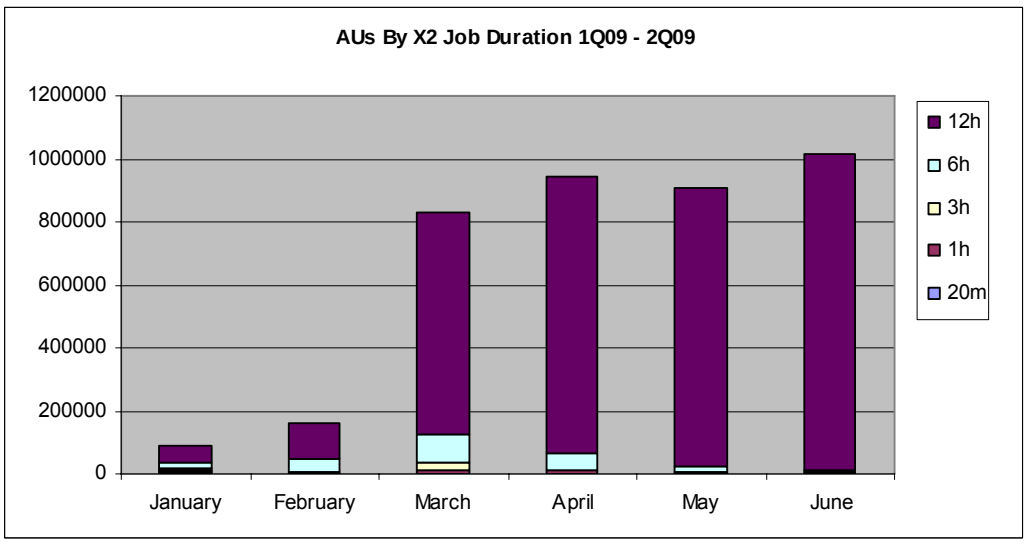
3.2.5 X2 Open Access Initiative

Accounting remained suspended on the X2 throughout 2Q09. Utilisation continued to rise throughout the quarter reaching a peak of 61% in June.

The graphs below illustrate the AU usage. It is clear that users have run both larger and longer jobs. In June, 99% of the AUs used on the X2 were as a result of jobs submitted to the 12 hour queues. 56% utilisation can be attributed to three main consortia - e01, e05 and e89

An additional 1.8M AUs were used in 2Q09 over 1Q09. This equates to a notional cost of approximately £906,000. The suspension of accounting on the X2 is due to end in August. In light of the success of the recent trial, a decision needs to be made on how to take this forward.





3.3. Performance Metrics

Metric	TSL(%)	FSL(%)	Apr-09	May-09	Jun-09	2Q09
Technology reliability (%)	85.00%	98.50%	99.1%	98.8%	98.2%	98.7%
Technology MTBF (hours)	100	126.4	244.0	366.0	244.0	274.5
Technology Throughput, hours/year	7000	8367	8534	8495	7346	8125
Capability jobs completion rate	70%	90%	100.0%	100.0%	97.7%	99.4%
Non in-depth queries resolved within 1 day (%)	85%	97%	98.8%	99.0%	99.3%	99.0%
Number of SP FTEs	7.3	8.0	8.6	8.9	10.1	9.2
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

4. Helpdesk

A total of 830 queries with a specified service metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	671	677	99.1%	97.0%
Admin queries finished in 1 day	592	596	99.3%	97.0%
Queries assigned in 30 min	827	830	99.6%	97.0%
Technical assessments in 10 days	18	19	94.7%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	366	44.1%
Admin	230	27.7%
In-depth	134	16.1%
Technical	81	9.8%
Technical assessment class-2	11	1.3%
Technical assessment class-1	8	1.0%

Queries by Category

Query Category	Queries	Percentage
New User	102	12.30%
3rd Party Software	98	11.80%
New Password	57	6.90%
Set user quotas	54	6.50%
Set group quotas	54	6.50%
User behaviour	50	6.00%
Access to HECToR	48	5.80%
New Group	46	5.50%
Node Failure	43	5.20%
Disk, tapes, resources	37	4.50%
Compilers and system software	37	4.50%
Batch system and queues	36	4.30%
Other	23	2.80%
User programs	22	2.70%
Login, passwords and ssh	22	2.70%
Add to group	22	2.70%
None	18	2.20%
Remove account	13	1.60%
Static website	10	1.20%
Join Project	10	1.20%
SAFE	9	1.10%
Courses	5	0.60%
Update account	4	0.50%

Performance and scaling	3	0.40%
Create certificate	2	0.20%
Porting	1	0.10%
Network	1	0.10%
Grid	1	0.10%
Delete from project	1	0.10%
Delete Certificate	1	0.10%

Queries by Handler Category

Handlers	Total	Automatic	In-depth	Admin	Technical assessment class-2	Technical	Technical assessment class-1	Percentage
OSG	441	366	12	22		41		53.13%
CSE	81		61		11	1	8	9.76%
USL	264		31	206		27		31.81%
Cray Systems	43		30	2		11		5.18%
Other	1					1		0.12%

5 System Hardware

5.1 HECToR Technology Changes

5.1.1 CLE2.1 Upgrade

The HECToR operating system was upgraded to CLE2.1 in May. Lessons learned from a previous attempt to complete the upgrade in March were implemented, resulting in a faster, more efficient upgrade.

Initially, it looked as if the upgrade to CLE 2.1 had worked perfectly, with the system passing its regression tests and being returned to service some hours early. However, within 24 hours we identified problems with a small number of user codes. A key issue was that the Unified Model would not recompile. This was not a problem with CLE 2.1 per se, rather it was caused by a change in the korn shell (ksh). Although the Unified Model did form part of the regression tests run by the CSE team, this was a preconfigured test case used for benchmarking which did not fully explore the "features" of the Makefile and hence did not uncover the problems. Some user-owned versions of codes would not run (including CASTEP and WRF). It transpired that these had not been recompiled despite repeated mailings to users on this.

A post-mortem was conducted by the service and lessons learned will be used for subsequent upgrades. Key recommendations included:

- More comprehensive regression testing
- More direct communications between the CSE team and key groups
- Access to the TDS for key consortia prior to major upgrades

These recommendations were adopted for the quad-core upgrade.

The operating system upgrade to CLE2.1 appears to have had a positive impact on the number of software related failures, with no failures of this type occurring in 2Q09.

5.1.2 Phase2a Quad-Core Upgrade

During June, the XT4 was upgraded from dual-core to quad-core processors. The hardware upgrade went very well with a number of additional Cray staff coming onsite from both the US and Europe to complete the task in hand. As well as the upgrade to quad-core processors, all 22,656 memory DIMMs were replaced, and all 60 cabinet blowers had rework completed on them. In total 28,320 components were swapped.

The hardware upgrade and testing went to plan with no major issues encountered. Preventative measures were taken by the team to ensure that the upgrade did not impact the live service. This planning was worthwhile as there was no impact on the main service as a result of the upgrade work which was taking place in parallel. Cray staff were also dedicated to supporting either the upgrade or the main service, and not both at the same time.

The upgrade to quad-core processors took place in two parts. During the first part, half of HECToR's dual-core processors were available to users (2832 processors). During the second part of the upgrade the same number of quad-core processors were made available for users (11,328 cores). On 19th June, 2832 quad-core nodes were made available to the

HECToR users. At this stage user accounting was disabled. Within 8 hours of the service moving to quad-core processors, there were over 100 quad-core jobs running. This was very positive and showed that the users had adopted quickly and changed scripts as required. The service was soon running at full capacity. On 29 June the remaining 2832 processors were brought online for users as quad-core. The service has been running at almost full capacity ever since, with utilisation at 95% in the period 19 - 30 June.

We have identified some issues on the quad-core architecture with the code 'Orb5' and there have also been some problems with some versions of VASP. The investigation into these is ongoing. Specific issues were identified with the chemistry code NWChem which could impact the availability of the HECToR service. A change to the environment in which NWChem jobs run was proven to fix this.

We can see that some users are choosing to run dual-core jobs. There may be cases where users require the additional memory on the processor. We are monitoring this and will be issuing reminder notes to users. The acceptance tests and availability trials have been scheduled for July. User accounting will be re-enabled once the availability trials have been completed.

5.2 Severity-1 Incidents

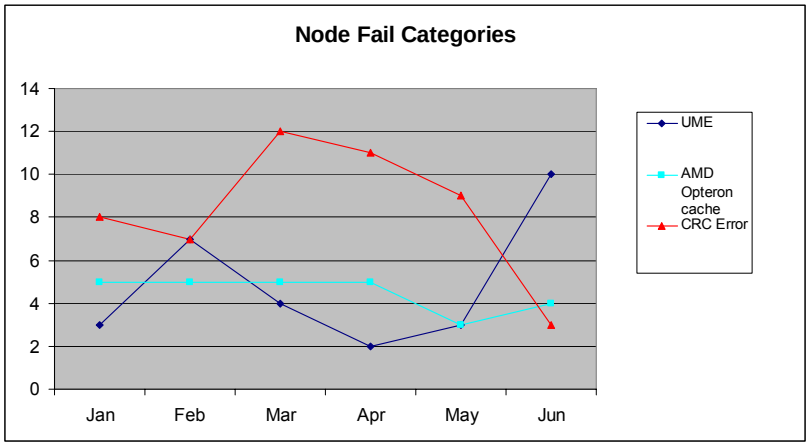
The monthly numbers of incidents and failures (SEV 1 incidents) are shown in the table below:

	April	***May***	***June***
Incidents	31	27	29
Failures	3	2	3

There were no service provision failures in 2Q09. Cray technology was responsible for the 8 Severity-1 incidents during 2Q09.Six of these incidents were due to hardware failures. Lustre related problems accounted for 1 Severity-1 incidents. On this occasion an overload of Lustre was directly linked to a user code. The user code has since been re-engineered however the exact reason why this impacted Lustre in the manner it did has not yet been proven. The final Severity-1 incident was as a result of a maintenance session which over-ran. The operating system upgrade to CLE2.1 appears to have had a positive impact on the number of software related failures, with no failures of this type occurring in 2Q09.

5.3 Single Node Failures

There were 68 single node failures in 2Q09 compared to 63 in 1Q09. The number of node failures as a result of Un-correctable memory error (dimm failures) increased in June. All 22,656 DIMMs were replaced during the Phase2a quad-core upgrade hence some initial failures are to be expected.



We will continue to monitor the rate of node failures throughout 3Q09.

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 Projects							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1	Dr Richard Blake	12,803,723	11,890,498	913,225
e01	UK Turbulence Consortium	EPSRC	Class1	Dr Gary N Coleman	3,107,500	1,913,347	1,194,153
e05	Materials Chemistry HPC Consortium	EPSRC	Class1	Prof C Richard A Catlow	1,129,327,228	12,610,724	1,116,656,504
e10	GENIUS	EPSRC	Class1	Prof Peter Coveney	9,257,856	5,458,088	3,799,768
e100	Large scale MD and quantum embedding for biological systems	EPSRC	Class2	Prof Zheng X Guo	100,000	27	99,973
e101	Optimization of HPCx LES code	EPSRC	Class2	Prof Michael Leschziner	100,001	18,502	81,499
e102	Numerical investigation of aerofoil noise	EPSRC	Class1	Dr Richard D Sandberg	5,000,000	1,383,167	3,616,833
e103	Micromagnetic simulations on HPC architectures	EPSRC	Class2	Dr Hans Fangohr	100,000	0	100,000
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1	Dr Nicolas Smiths	2,400,000	0	2,400,000
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1	Dr Andreas M Kempf	1,300,000	0	1,300,000
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1	Prof Kai Luo	3,650,000	0	3,650,000
e107	Parallel Brain Surgery Simulation	EPSRC	Class1	Dr Stephane P. A. Bordas	6,000,000	5	5,999,995
e108	Unsteady Propeller Noise	EPSRC	Class2	Dr Sergey Karabasov	100,000	0	100,000

e110	Computational Aeroacoustics Consortium	EPSRC	Class1	Prof Paul Tucker	39,100,000	1,486,380	37,613,620
e112	Assessment of the ONETEP code	EPSRC	Class2	Mr Andrew J Scott	100,000	0	100,000
e113	[dCSE] MRBV ? Massive Remove Batch Visualizer	EPSRC	Class2	Dr Martin Turner	85,440	0	85,440
e114	[dCSE] OpenFOAM	EPSRC	Class2	Mr Paul Graham	100,000	0	100,000
e115	Multiscale Modelling of Biological Systems	EPSRC	Class2	Prof Jonathan W Essex	100,000	0	100,000
e116	Scaling and Benchmarking Spectral Codes	EPSRC	Class2	Dr Benson Muite	100,000	864	99,136
e117	Getting started on HECTOR	EPSRC	Class2	Dr Carmen Domene	100,000	0	100,000
e118	Adaptive coupled radiation-transport and fluids modelling.	EPSRC	Class2	Prof Christopher Pain	100,000	0	100,000
e119	Nanoscale Energy Transportation	EPSRC	Class2	Dr Dongsheng Wen	100,000	0	100,000
e120	[dCSE] FF Transformations for plasma simulations	EPSRC	Class2	Dr Colin M Roach	200,000	0	200,000
e121	[dCSE] Improving Performance using Wannier functions	EPSRC	Class2	Prof Maria Merlyne DeSouza	200,000	0	200,000
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1	Dr Colin M Roach	65,000,000	155,772	64,844,228
e123	Finger-jets and turbulent structures	EPSRC	Class2	Dr David Ingram	15,040	0	15,040
e124	Compressible Axisymmetric Flows	EPSRC	Class1	Dr Richard D Sandberg	15,000,000	0	15,000,000
e125	Fermion Monte Carlo in Slater Determinant spaces	EPSRC	Class2	Dr Ali Alavi	100,000	0	100,000
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1	Dr Xi Jiang	9,984,000	0	9,984,000
e24	DEISA	EPSRC	Class1	Mrs Alison Kennedy	42,323,067	12,163,535	30,159,532

e34	Hydrogen vacancy distribution in magnesium hydride	EPSRC	Class2	Prof Nora de Leeuw	100,000	18,081	81,919
e35	Non-adiabatic processes	EPSRC	Class1	Dr Tchavdar Todorov	3,000,000	275,491	2,724,509
e42	Computational Combustion for Engineering Applications	EPSRC	Class1	Prof Kai Luo	32,000,001	7,968,856	24,031,145
e59	Turbulence in Breaking Gravity Waves	EPSRC	Class1	Prof Ian P Castro	708,922	440,737	268,185
e63	UK Applied Aerodynamics Consortium 2	EPSRC	Class1	Dr Nick Hills	13,500,000	6,975,934	6,524,066
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1	Dr Angelos Michaelides	50,000,000	24,493,166	25,506,834
e69	Simulations of a Subsonic Cylindrical Cavity Flow	EPSRC	Class2	Dr Aldo Rona	125,001	125,273	-272
e70	Computation of Electron Transfer Properties	EPSRC	Class1	Dr Jochen Blumberger	960,000	257,619	702,381
e71	Simulating the control of calcite crystallisation	EPSRC	Class1	Prof John Harding	40,266,342	40,203,133	63,209
e72	Ultrascalable Modelling of Materials	EPSRC	Class2	Dr Lee Margetts	8,622,547	8,459,578	162,969
e74	Quantum Monte Carlo Methods	EPSRC	Class1	Prof Dario Alfe`	30,008,735	32,477,320	-2,468,585
e75	Terascale DNS of Turbulence	EPSRC	Class1	Prof Christos Vassilicos	27,881,305	27,781,306	99,999
e76	HELIUM Developments	EPSRC	Class1	Prof Ken Taylor	6,058,305	6,058,303	2
e77	Porting of DFT/GW Codes	EPSRC	Class2	Prof Maria Merlyne DeSouza	160,000	60,676	99,324
e79	SMEAGOL	EPSRC	Class1	Prof Colin Lambert	3,000,000	36	2,999,964
e81	e-Collision experiments using HPC	EPSRC	Class2	Prof NS Scott	200,000	607	199,393
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class2	Dr Peter Haynes	100,000	90,798	9,202

e84	Vortical Mode Interactions	EPSRC	Class1	Dr Tamer Zaki	9,600,000	1,989	9,598,011
e85	Study of Interacting Turbulent Flames	EPSRC	Class1	Dr N Swaminathan	5,588,610	6,192	5,582,418
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1	Dr Matt Probert	360,000,001	38,961,284	321,038,717
e90	Network modelling of wireless cities	EPSRC	Class2	Prof Jonathan M Pitts	100,000	22,947	77,053
e92	Dynamo Action In Compressible Convection	EPSRC	Class2	Mr Paul Bushby	75,000	74,433	567
e94	Porting the Linear Scaling DTF Code Conquest to HECToR	EPSRC	Class2	Dr David Bowler	100,000	112,043	-12,043
e96	Materials Property Relationships	EPSRC	Class2	Dr Shoufeng Yang	100,000	0	100,000
e98	Non-linear magnetohydrodynamic modelling of tokamak plasmas	EPSRC	Class2	Mr Ian T Chapman	100,000	26,287	73,713
u02	Materials simulation using AIMPRO	EPSRC	Early use	Dr Patrick R Briddon	4,000,000	3,080,443	919,557
u03	DNS of NACA-0012 aerofoil at Mach 0.4	EPSRC	Early use	Dr Gary N Coleman	2,500,000	2,301,060	198,940
u10	Turbulent Plasma Transport in Tokamaks	EPSRC	Early use	Dr Colin M Roach	2,500,000	2,393,739	106,261
y08	Testing	EPSRC	Early use	Dr David Jenkins	1,000	0	1,000
NERC projects							
n01	Global Ocean Modelling Consortium	NERC	Class1	Dr Thomas Anderson	19,343,840	8,571,824	10,772,016
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1	Dr Lois Steenman-Clark	121,032,034	44,002,745	77,029,289
n03	Computational Mineral Physics Consortium	NERC	Class1	Prof John P Brodholt	150,618,316	71,182,686	79,435,630
n04	Shelf Seas Consortium	NERC	Class1	Dr Roger Proctor	39,009,435	5,209,435	33,800,000

BBSRC projects							
b01	Biomarkers for patient classification	BBSRC	Class2	Prof. Peter Ghazal	100,000	300,794	-200,794
b08	Int BioSim	BBSRC	Class1	Mr Mark M Sansom	866,000	44,101	821,899
b09	Circadian Clock	BBSRC	Class1	Prof Andrew A Millar	2,000,000	0	2,000,000
STFC projects							
p01	Atomic Physics for APARC	STFC	Class1	Dr Penny Scott	3,020,000	0	3,020,000
External projects							
x01	HPC-Europa	External	Class1	Dr Judy Hardy	2,183,338	1,132,022	1,051,316
x02	BlueArc (TDS)	External	Service	Mr M W Brown	1,000	0	1,000
T01	NIMES: New Improved Muds from Environmental Sources.	External	Class1	Dr Chris Greenwell	4,113,669	190,883	3,922,786
Director's Time							
y09	Director's Time	DirectorsTime	Service	Prof Arthur S Trew	846,708	82,538	764,170
d03	EUFORIA	DirectorsTime	Service	Mr Adrian Jackson	2,200,000	766,787	1,433,213
d04	MSc Projects	DirectorsTime	Service	Dr David Henty	93,500	33,227	60,273
d07	Thermal ellipsiods and proton transfer	DirectorsTime	Service	Dr Carole A Morrison	1,116,000	369,934	746,066
d08	Oncology	DirectorsTime	Service	Mr Paul Graham	35,000	25,531	9,469
d09	ICHEC	DirectorsTime	Class2	Dr Jean-Christophe Desplat	1,000,000	456,748	543,252