



HECToR Quarterly Report

April – June 2008

1. Introduction

This report covers the period from 1 April 2008 at 0800 to 1 July 2008 at 0800.

Section 2 summarises service availability and performance statistics for this quarter. Section 3 shows utilisation of the service for the last six months. Section 4 shows Helpdesk statistics. 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/2Q08.php>

2. Executive Summary

- Utilisation has continued to improve in 2Q08, with the quarterly average increasing from just over 50% in 1Q08 to nearly 80% in 2Q08. Utilisation from EPSRC funded projects has more than doubled from 31% to 65% quarter on quarter. The capability challenge projects have again contributed significantly to this increase. A number of dormant EPSRC Class 2 projects have been identified where no AUs have yet been used, and follow up is in progress with PIs to understand why. NERC utilisation has decreased slightly overall, although n02 usage is on the rise. An additional 170 user accounts were created in total during 2Q08, bringing the total user count to 489.
- The number of failures during 2Q08 remained disappointing with a decrease in the average reliability from 1Q08. One particular failure in June as a result of a security alert had a significant effect on the overall statistics, as it resulted in 15 hours unplanned downtime. On a more positive note the MTBF improved slightly on 1Q08 from 146 to 169 hours.
- There was a 16% increase in the volume of queries to the helpdesk, with 908 queries being raised in total in 2Q08. Despite the increase in volume the associated helpdesk targets were surpassed in most areas. The increase in queries was primarily in the administrative category, whilst the volume of technical and in-depth queries remained comparable to the previous quarter.

3. Availability

Failures

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

	<i>April</i>	<i>May</i>	<i>June</i>
Incidents	38	38	28
Failures	6	2	5

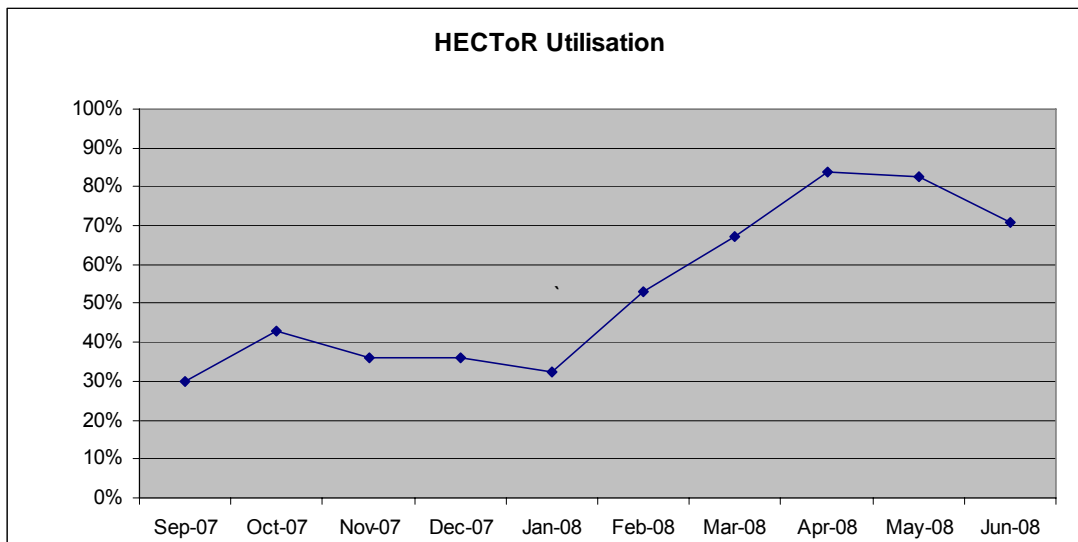
Performance Statistics

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

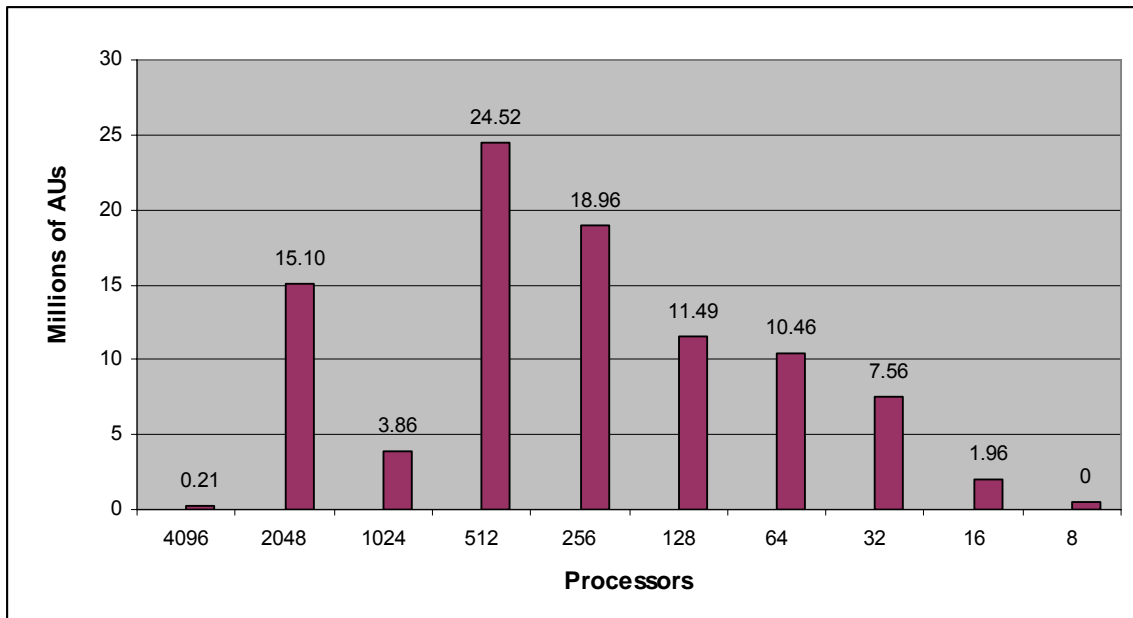
<i>Attribution</i>	<i>Metric</i>	<i>April</i>	<i>May</i>	<i>June</i>	<i>Quarterly</i>
Technology	Failures	6	2	5	13
	MTBF	122	366	146	169
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	6	2	5	13
	MTBF	122	366	146	169

4. HECToR Utilisation

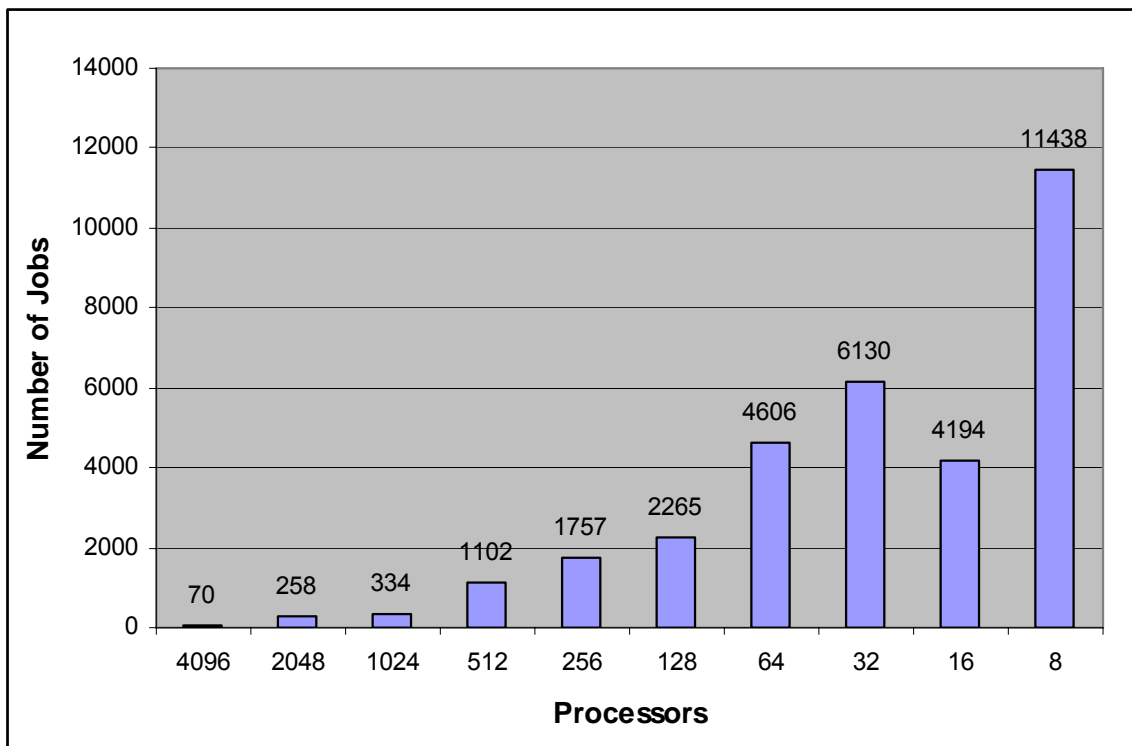
Overall Utilisation



Utilisation by queue



Number of jobs per queue



Usage by Consortium

Project	AUs	NJobs	%age of Use	Utilisation
c01	2,929,972	1201	3.1%	2.5%
e05	8,212	37	0.0%	0.0%
e10	101,815	837	0.1%	0.1%
e24	634,192	308	0.7%	0.5%
e35	1,238	51	0.0%	0.0%
e42	436,138	513	0.5%	0.4%
e63	774,460	179	0.8%	0.6%
e68	5,614,964	3417	5.9%	4.7%
e69	22,507	67	0.0%	0.0%
e71	22,608,968	1955	23.9%	18.9%
e72	1,665,008	508	1.8%	1.4%
e73	787,626	191	0.8%	0.7%
e74	16,144,512	2216	17.1%	13.5%
e75	9,339,717	518	9.9%	7.8%
e77	18,022	221	0.0%	0.0%
e78	1,344	13	0.0%	0.0%
e79	19	9	0.0%	0.0%
e80	13,672,420	168	14.5%	11.5%
e83	35,748	21	0.0%	0.0%
e84	16	11	0.0%	0.0%
e86	103,105	21	0.1%	0.1%
e88	2,161,514	307	2.3%	1.8%
e89	831,591	713	0.9%	0.7%
e92	0	1	0.0%	0.0%
e93	277,843	361	0.3%	0.2%
e94	694	12	0.0%	0.0%
u02	55,269	128	0.1%	0.0%
u10	49,672	377	0.1%	0.0%
EPSRC Total	78,276,589	14361	82.7%	65.6%
n01	995,442	1235	1.1%	0.8%
n02	6,279,000	4664	6.6%	5.3%
n03	7,648,773	3558	8.1%	6.4%
n04	55,235	143	0.1%	0.0%
u07	2,463	10	0.0%	0.0%
NERC Total	14,980,912	9610	15.8%	12.6%
u04	900,021	338	1.0%	0.8%
BBSRC Total	900,021	338	1.0%	0.8%
x01	56,586	400	0.1%	0.0%
External Total	56,586	400	0.1%	0.0%
d01	48,564	30	0.1%	0.0%
d03	9,847	379	0.0%	0.0%
d04	7,604	208	0.0%	0.0%
DirectorsTime Total	66,014	617	0.1%	0.1%
y01	0	1820	0.0%	0.0%
y02	65,906	777	0.1%	0.1%

y03	0	57	0.0%	0.0%
y04	26	14	0.0%	0.0%
y05	0	1	0.0%	0.0%
y06	4	1033	0.0%	0.0%
z01	172,426	705	0.2%	0.1%
z02	37,730	304	0.0%	0.0%
z03	49,851	2209	0.1%	0.0%
Internal Total	325,944	6920	0.3%	0.3%
Total	94,606,068	32246	100.0%	79.3%

5. Helpdesk

A total of 908 queries with a specified service metric were completed in this period.

Helpdesk targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	761	763	100%	97%
Admin queries finished in 1 day	682	684	100%	97%
Queries assigned in 30 min	895	908	99%	97%
Technical assessments in 10 days	19	22	86%	97%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	493	53.3%
Admin	191	20.6%
In-depth	123	13.5%
Technical	79	8.7%
Technical assessment class-1	15	1.7%
Technical assessment class-2	7	0.8%

Queries by Category

Query Category	Queries	Percentage
New User	169	18.6%
Set group quotas	86	9.5%
None	77	8.5%
Add to group	73	8%
Access to HECToR	66	7.3%
New Password	59	6.5%
Set user quotas	54	5.9%
Disk, tapes, resources	39	4.3%
Other	38	4.2%
Compilers and system software	38	4.2%
3rd Party Software	37	4.1%
New Group	32	3.5%
Batch system and queues	32	3.5%
Login, passwords and ssh	23	2.5%
Join Project	15	1.7%
SAFE	14	1.5%

User behaviour	12	1.3%
User programs	10	1.1%
Performance and scaling	8	0.9%
Courses	7	0.8%
Delete from group	6	0.7%
Create certificate	4	0.4%
Static website	3	0.3%
Remove account	3	0.3%
Porting	2	0.2%
Grid	1	0.1%

Queries by Handler category

Handlers	Total	Automatic	In-depth	Admin	Technical	Technical assessment class-1	Technical assessment class-2	Percentage
OSG	561	493	12	25	31			61.8%
CSE	66		48	1	1	14	2	7.3%
USL	254		46	159	43	1	5	28%
Other	9		1	5	3			1%
Cray Systems	18		16	1	1			2%

6. Summary of Performance Metrics

Metric	TSL(%)	FSL(%)	Apr-08	May-08	Jun-08	2Q08
Technology reliability (%)	85.0%	98.5%	94.5	99.3	96.6	96.8
Technology MTBF (hours)	100.0	126.4	122.0	366.0	146.4	169
Technology Throughput, hours/year	7000	8367	8205	8551	7750	8169
Capability jobs completion rate	70%	90%	95.2	97.9	93.3	95.7
Non in-depth queries resolved within 1 day (%)	85%	97%	100.0	100.0	100.0	100.0
Number of SP FTEs	7.25	8.0	8.0	8.2	8.3	8.2
SP serviceability (%)	80.0%	99.0%	100.0	100.0	100.0	100.0

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

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	Class	Area	PI	Total AUs allocated	AUs used	AUs left
EPSRC projects							
T01	NIMES: New Improved Muds from Environmental Sources.	Class1	Environment	Dr Chris Greenwell	4,113,669	0	4,113,669
c01	Support of EPSRC/STFC SLA	Class1	support	Dr Richard Blake	12,803,723	5,699,970	7,103,753
d01	UKQCD-DT	Early use	Physics	Dr Jonathan Flynn	4,007,024	3,963,747	43,277
d02	HELIUM-DT	Early use	Physics	Prof Ken Taylor	3,067,442	3,067,443	-1
d03	EUFORIA	Service	Physics	Mr Adrian Jackson	1,000,000	9,847	990,153
d04	MSc Projects	Service	External	Dr David Henty	100,000	7,608	92,392
e01	UK Turbulence Consortium	Class1	Engineering	Dr Gary N Coleman	2,707,500	0	2,707,500
e05	Materials Chemistry HPC Consortium	Class1	Chemistry	Prof C R A Catlow	1,129,257,228	9,169	1,129,248,059
e10	GENIUS	Class1	Chemistry	Prof Coveney	4,500,000	101,815	4,398,185
e24	DEISA	Class1	support	Mrs A Kennedy	12,853,334	634,192	12,219,142
e34	Hydrogen vacancy distribution in magnesium hydride	Class2	Chemistry	Prof Nora de Leeuw	100,000	0	100,000
e35	Non-adiabatic processes	Class1	Materials	Dr T Todorov	1,000,000	1,436	998,564
e42	Computational Combustion for Engineering Applications	Class1	Engineering	Prof Kai Luo	32,000,000	2,230,691	29,769,309
e63	UK Applied Aerodynamics Consortium 2	Class1	Engineering	Dr Nick Hills	13,500,000	975,448	12,524,552
e68	Hydrogenation Reactions at Metal Surfaces	Class1	Chemistry	Dr Angelos Michaelides	50,000,000	8,754,735	41,245,265

e69	Simulations of a Subsonic Cylindrical Cavity Flow	Class2	Engineering	Dr Aldo Rona	100,000	22,807	77,193
e70	Computation of Electron Transfer Properties	Class1	Chemistry	Dr Jochen Blumberger	960,000	86	959,914
e71	Simulating the control of calcite crystallisation	Class1	Chemistry	Prof John Harding	40,000,000	30,830,665	9,169,335
e72	Ultrascale Modelling of Materials	Class1	Materials	Dr Lee Margetts	27,660,000	1,684,212	25,975,788
e73	Tera-scale Shear Flow Challenge	Class1	Materials	Dr Kevin Stratford	15,800,000	3,752,345	12,047,655
e74	Quantum Monte Carlo Methods	Class1	Materials	Prof Dario Alfe`	30,000,000	29,156,176	843,824
e75	Terascale DNS of Turbulence	Class1	Engineering	Prof Christos Vassilicos	27,520,000	13,148,857	14,371,143
e76	HELIUM Developments	Class1	Physics	Prof Ken Taylor	6,000,000	0	6,000,000
e77	Porting of DFT/GW Codes	Class2	Engineering	Prof Maria Merlyne DeSouza	60,000	29,753	30,247
e78	Q-Espresso CP/PWSCF Codes on HECToR	Class2	Chemistry	Dr Antonio Tilocca	100,000	52,535	47,465
e79	SMEAGOL	Class1	Physics	Prof Colin Lambert	2,960,000	20	2,959,980
e80	Double Ionisation of Helium	Class1	Physics	Prof Ken Taylor	30,000,000	16,851,721	13,148,279
e81	e-Collision experiments using HPC	Class2	Physics	Prof NS Scott	200,000	0	200,000
e82	ONETEP: linear-scaling method on High Performance Computers	Class2	Materials	Dr Peter Haynes	100,000	0	100,000
e83	Ab initio study of high pressure disordered ice	Class2	Physics	Dr Simon P Bates	100,000	35,748	64,252
e84	Vortical Mode Interactions	Class1	Engineering	Dr Tamer Zaki	3,200,000	16	3,199,984
e85	Study of Interacting Turbulent Flames	Class1	Engineering	Dr N Swaminathan	2,083,000	0	2,083,000
e86	Single molecule vibrational microscopy and spectroscopy	Class2	Materials	Prof Andrew Fisher	100,000	103,105	-3,105

e87	Model Parameters for Unsaturated Elasto-plastic Models	Class2	Engineering	Dr Charles Augarde	100,000	0	100,000
e88	Molecular Dynamics Simulation of a protein-ligand complex	Class1	Chemistry	Dr Charles Laughton	10,000,000	2,197,788	7,802,212
e89	Support for UK Car-Parrinello Consortium	Class1	Physics	Dr Matt Probert	140,000,000	851,671	139,148,329
e90	Network modelling of wireless cities	Class2	Engineering	Prof Jonathan M Pitts	100,000	0	100,000
e91	Bulk properties of TiO ₂ -B as lithium battery anodes	Class2	Chemistry	Prof M Saiful Islam	100,000	0	100,000
e92	Dynamo Action In Compressible Convection	Class2	Physics	Mr Paul Bushby	75,000	0	75,000
e93	ACE - Architecture Exercise	Service	support	Dr Lorna Smith	300,000	290,099	9,901
e94	Porting the Linear Scaling DTF Code Conquest to HECToR	Class2	Physics	Dr David Bowler	100,000	1,002	98,998
e95	Novel Apatite Materials	Class2	Materials	Prof M Saiful Islam	100,000	0	100,000
e96	Materials Property Relationships	Class2	Materials	Dr Shoufeng Yang	100,000	0	100,000
u02	Materials simulation using AIMPRO	Early use	Materials	Dr Patrick R Briddon	4,000,000	3,061,126	938,874
u03	DNS of NACA-0012 aerofoil at Mach 0.4	Early use	Engineering	Dr Gary N Coleman	2,500,000	2,286,958	213,042
u06	Modelling of Protein Flexibility Upon Ligand Binding	Early use	Chemistry	Prof Jonathan W Essex	1,900,000	1,906,861	-6,861
u08	UKQCD	Early use	Physics	Dr Jonathan Flynn	8,000,000	7,969,011	30,989
u09	Laser Double Ionization of Helium at 800 nm	Early use	Physics	Prof Ken Taylor	6,000,000	6,215,035	-215,035
u10	Turbulent Plasma Transport in Tokamaks	Early use	Physics	Dr Colin M Roach	2,500,000	1,645,811	854,189
u11	Ice Nucleation and Growth	Early use	Environment	Prof Mark Rodger	1,000,000	993,256	6,744

NERC Projects							
n01	Global Ocean Modelling Consortium	Class1	Environment	Dr Thomas Anderson	9,500,000	2,738,114	6,761,886
n02	NCAS (National Centre for Atmospheric Science)	Class1	Environment	Dr Lois Steenman-Clark	51,750,000	10,139,405	41,610,595
n03	Computational Mineral Physics Consortium	Class1	Environment	Prof John P Brodholt	72,529,000	31,934,183	40,594,817
n04	Shelf Seas Consortium	Class1	Environment	Dr Roger Proctor	8,250,000	70,895	8,179,105
u01	Melting of MgSiO ₃ Perovskite	Early use	Environment	Prof John P Brodholt	11,000,000	11,018,423	-18,423
u05	OCEANS 2025	Early use	Environment	Dr Thomas Anderson	600,000	32,440	567,560
u07	NCAS	Early use	Environment	Dr Lois Steenman-Clark	2,000,000	131,438	1,868,562
BBSRC Projects							
u04	Biomolecular simulation code performance	Early use	Life Sciences	Dr Charles Laughton	7,000,000	2,523,361	4,476,639
External projects							
x01	HPC-Europa	Class1	External	Dr Judy Hardy	375,000	111,114	263,886
Directors Time							
d01	UKQCD-DT	Early use	Physics	Dr Jonathan Flynn	4,007,024	3,963,747	43,277
d02	HELIUM-DT	Early use	Physics	Prof Ken Taylor	3,067,442	3,067,443	-1
d03	EUFORIA	Service	Physics	Mr Adrian Jackson	1,000,000	9,847	990,153
d04	MSc Projects	Service	External	Dr David Henty	100,000	7,608	92,392
y09	Director's Time	Service	External	Prof Arthur S Trew	82,538	82,538	0