



HECToR Quarterly Report

January – March 2008

1. Introduction

This report covers the period from 1 January 2008 at 0800 to 1 April 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/1Q08.php>

2. Executive Summary

- Utilisation has continued to increase during Q1_08 with a ramp from 32% in January to 67% in March. The Capability Challenge projects (in particular e74) and project n03 have contributed significantly to this.
- As yet there is no sign of improvement in the number of failures/MTBF. A number of open issues remain with Cray for analysis. Software related failures dominate the more recent failures.
- 784 queries were raised in total during Q1_08 and the associated helpdesk targets for the period were exceeded in most areas.

3. Availability

Failures

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

	<i>January</i>	<i>February</i>	<i>March</i>
Incidents	24	35	25
Failures	5	7	5

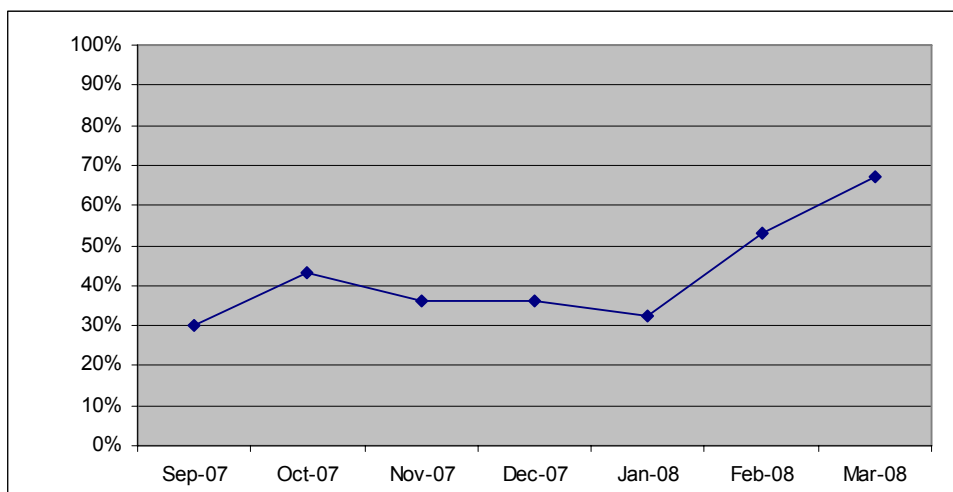
Performance Statistics

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

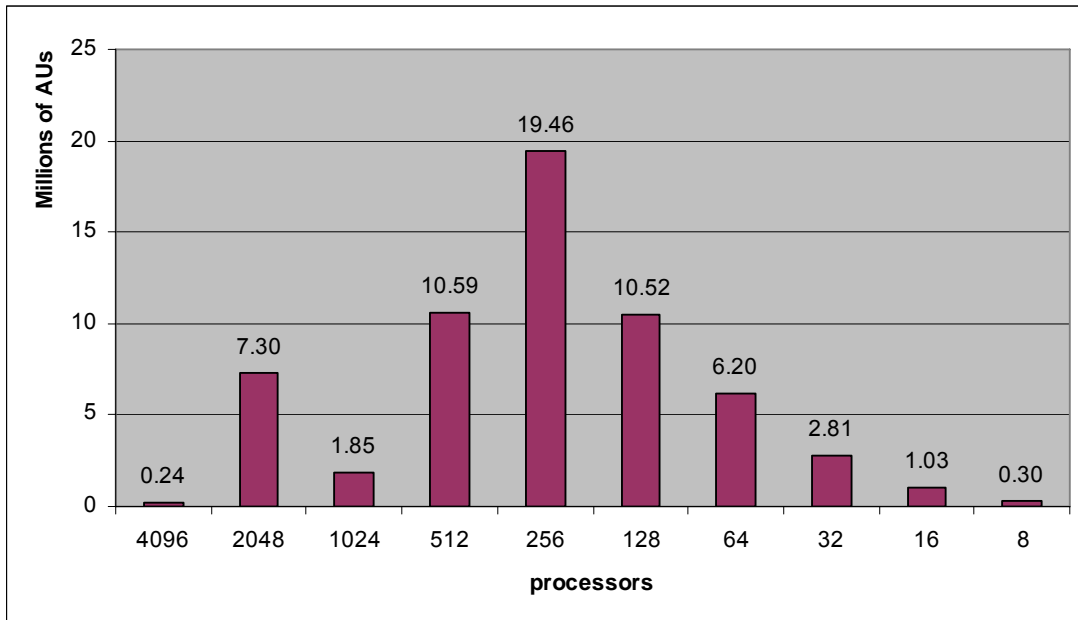
<i>Attribution</i>	<i>Metric</i>	<i>January</i>	<i>February</i>	<i>March</i>	<i>Quarterly</i>
Technology	Failures	4	7	4	15
	MTBF	183	105	183	146
Service Provision	Failures	1	0	0	1
	MTBF	732	∞	∞	2196
External	Failures	0	0	1	1
	MTBF	∞	∞	732	2196
Overall	Failures	5	7	5	17
	MTBF	146	105	146	129

4. HECToR Utilisation

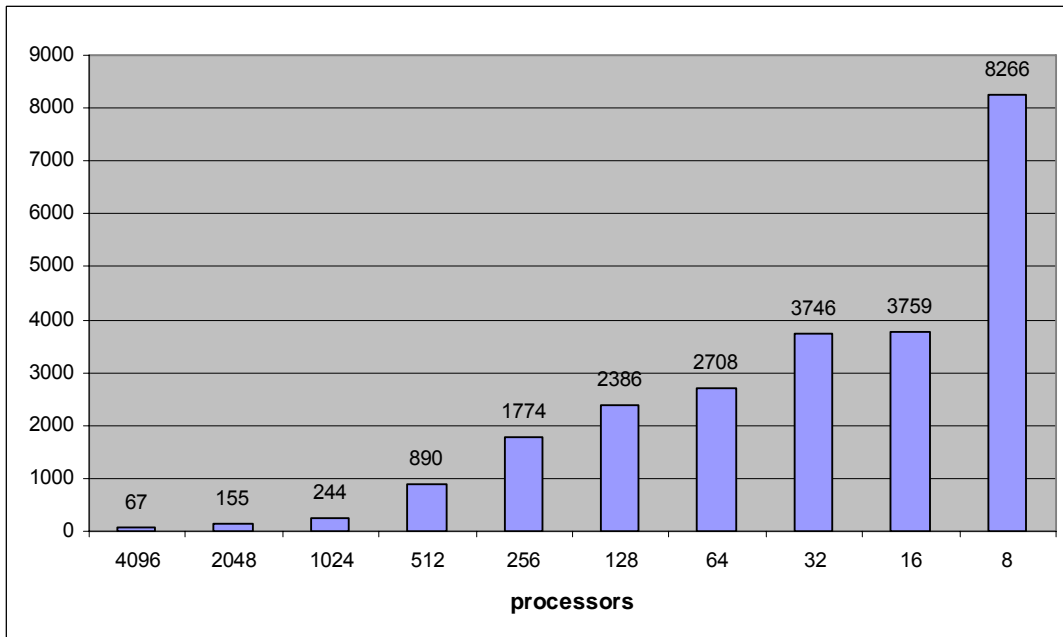
Overall Utilisation



Utilisation by queue



Number of jobs per queue



Usage by Consortium

Project	AUs	NJobs	%age of Use	Utilisation
c01	2,663,455	2632	4.4%	2.2%
e35	198	27	0.0%	0.0%
e42	160,481	240	0.3%	0.1%
e63	196,921	74	0.3%	0.2%
e68	2,995,660	1900	5.0%	2.5%
e69	275	168	0.0%	0.0%
e71	7,889,326	1644	13.1%	6.6%
e72	18,771	326	0.0%	0.0%
e73	2,960,066	163	4.9%	2.5%
e74	12,930,689	1647	21.4%	10.8%
e75	3,750,099	358	6.2%	3.1%
e77	11,731	120	0.0%	0.0%
e78	51,191	68	0.1%	0.0%
e79	0	26	0.0%	0.0%
e80	3,175,829	42	5.3%	2.7%
u02	73,331	49	0.1%	0.1%
u03	343,085	21	0.6%	0.3%
u10	165,186	572	0.3%	0.1%
EPSRC Total	37,386,296	10077	62%	31.3%
n01	1,116,658	939	1.9%	0.9%
n02	2,784,980	2520	4.6%	2.3%
n03	15,885,905	4941	26.3%	13.3%
n04	15,660	339	0.0%	0.0%
u07	10,869	43	0.0%	0.0%
NERC Total	19,814,072	8782	32.9%	16.6%
u04	814,147	211	1.4%	0.7%
BBSRC Total	814,147	211	1.4%	0.7%
x01	54,528	548	0.1%	0%
External Total	54,528	548	0.1%	0%
d01	808,159	74	1.3%	0.7%
d02	1,138,659	39	1.9%	1.0%
d03	0	2	0.0%	0.0%
d04	1	5	0.0%	0.0%
DirectorsTime Total	1,946,819	120	3.2%	1.6%
y02	210,277	807	0.3%	0.2%
y03	2,731	163	0.0%	0.0%
y04	1,554	22	0.0%	0.0%
y05	12,641	902	0.0%	0.0%
z01	18,928	838	0.0%	0.0%
z02	9,432	205	0.0%	0.0%
z03	19,137	1321	0.0%	0.0%
Internal Total	274,701	4258	0.5%	0.2%
TOTAL:	60,290,562	23996	100%	50.50%

5. Helpdesk

A total of 784 queries with a specified service metric were completed in this period.

Helpdesk targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	632	634	100%	97%
Admin queries finished in 1 day	561	562	100%	97%
Queries assigned in 30 min	771	784	98%	97%
Technical assessments in 10 days	23	25	92%	97%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	448	57.1%
In-depth	125	15.9%
Admin	114	14.5%
Technical	72	9.2%
Technical assessment	25	3.2%

Queries by Category

Query Category	Queries	Percentage
Set user quotas	138	17.6%
New User	108	13.8%
Set group quotas	102	13.0%
New Password	55	7.0%
Disk, tapes, resources	55	7.0%
Access to HECToR	50	6.4%
Batch system and queues	46	5.9%
Compilers and system software	40	5.1%
None	29	3.7%
3rd Party Software	27	3.4%
New Group	24	3.1%
Other	23	2.9%
Add to group	16	2.0%
SAFE	12	1.5%
Login, passwords and ssh	12	1.5%

Join Project	12	1.5%
User behaviour	8	1.0%
User programs	5	0.6%
Performance and scaling	5	0.6%
Grid	4	0.5%
Porting	3	0.4%
Network	3	0.4%
Create certificate	3	0.4%
Static website	2	0.3%
Delete from group	1	0.1%
Courses	1	0.1%

Queries by Handler category

Handlers	Total	Automatic	In-depth	Admin	Technical	Technical assessment	Percentage
OSG	531	448	32	18	33		67.7%
CSE	65		36	3	3	23	8.3%
Cray Systems	24		20	1	3		3.1%
USL	145		35	76	32	2	18.5%
Other	19		2	16	1		2.4%

6. Summary of Performance Metrics

Metric	TSL(%)	FSL(%)	Jan-08	Feb-08	Mar-08	1Q08
Technology reliability (%)	85.0%	98.5%	98.6	97.8	98.8	98.4
Technology MTBF (hours)	100.0	126.4	183	105	183	146.4
Technology Throughput, hours/year	7000	8367	8771	8766	8761	8766
Capability jobs completion rate	70%	90%	93.5	97.0	98.0	96.2
Non in-depth queries resolved within 1 day (%)	85%	97%	99	100	99	99
Number of SP FTEs	7.25	8.0	8.8	7.9	8.0	8.2
SP serviceability (%)	80.0%	99.0%	99.9	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	Class	Title	PI
EPSRC Projects			
e01	1	UK Turbulence Consortium	Dr Gary Coleman
e10	1	GENIUS:Grid Enabled Neurosurgical Imaging Using Simulation	Prof Peter Coveney
e42	1	Consortium on Computational Combustion for Engineering Applications	Prof K Luo
e35	1V	Non-Adiabatic Processes	Dr Tchavdar Todorov
e63	1	Supercomputing resources and Support for the UK Applied Aerodynamics Consortium 2 (2007-2010)	Dr Nick Hills
e68	1	Hydrogenation Reactions at Metal Surfaces	Dr A Michaelides
e69	2	Simulations of a Subsonic Cylindrical Cavity Flow	Dr Aldo Rona
e70	1	Computation of Electron Transfer Properties	Dr Jochen Blumberger
e71	1	Simulating the control of calcite crystallisation	Prof John Harding
e72	1	Ultrascale Modelling of Materials	Dr Lee Margetts
e73	1	Tera-scale Shear Flow Challenge	Dr Kevin Stratford
e74	1	Quantum Monte Carlo Methods	Dr Dario Alfe
e75	1	Terascale DNS of Turbulence Generated by Fractal Grids	Prof Christos Vassilicos
e76	1	HELIUM Developments	Prof Ken Taylor
e77	2	Porting of DFT/GW Codes - ab init, EXC, PWSCF and GWW	Prof Maria Merlyne DeSouza
e78	2	Q-Espresso CP/PWSCF Codes on HECToR	Dr A Tilocca
e79	1	SMEAGOL	Prof Colin Lambert
e80	1	Double Ionisation of Helium	Prof Ken Taylor
e81	2	e-Collision experiments using HPC	Prof NS Scott
e82	2	ONETEP: linear-scaling method on High Performance Computers	Prof Peter Haynes
e83	2	Ab initio study of high pressure disordered ice	Dr Simon Bates
e84	1	Vortical Mode Interactions	Dr Tamer Zaki
e85	1	Study of Interacting Turbulent Flames	Dr N Swaminathan
e86	2	Single molecule vibrational microscopy and spectroscopy	Prof Andrew Fisher
e87	2	Identification of model parameters for unsaturated elasto-plastic models from pressuremeter tests using parallel computing	Dr Charles Augarde
e88	1	The First Super-Microsecond Molecular Dynamics Simulation of a Protein-Ligand complex: MUP/IBM	Dr Charles Laughton
u02	e	Materials simulation using AIMPRO	Dr Patrick R Briddon
u03	e	DNS of NACA-0012 aerofoil at Mach 0.4: u03	Dr Gary N Coleman

u06	e	Modelling of Protein Flexibility Upon Ligand Binding: u06	Prof Jonathan W Essex
u08	e	UKQCD	Dr Jonathan Flynn
u09	e	Laser Double Ionization of Helium at 800 nm: u09	Prof Ken Taylor
u10	e	Turbulent Plasma Transport in Tokamaks	Dr Colin M Roach
u11	e	Ice Nucleation and Growth	Prof Mark Rodger
c01	1	Support of EPSRC/STFC SLA	Dr Richard Blake

NERC Projects			
n01	1	Large-Scale Long-Term Ocean Circulation	Dr Thomas Anderson
n02	1	NCAS	Dr Lois Steenman-Clark
n03	1	Computational Mineral Physics Consortium	Prof John Brodholt
n04	1	Shelf Seas Consortium	Dr Roger Proctor
u05	e	OCEANS 2025	Mrs Beverly de Cuevas
u07	e	NCAS	Dr Lois Steenman-Clark
u01	e	Melting of MgSiO ₃ Perovskite	Prof John P Brodholt

BBSRC			
u04		Biomolecular simulation code performance: u04	Dr Charles Laughton

External Projects			
x01	External	HPC-Europa	Dr Judy Hardy
Directors' Time			
d01		UKQCD-DT (Directors time for UKQCD)	Dr Jonathan Flynn
d02		HELIUM-DT (Directors time for Helium)	Dr Ken Taylor
d03		EUFORIA	Mr Adrian Jackson
d04		MSc Projects	Dr David Henty