HECToR Quarterly Report

Jul - Sep 2012

1   Introduction

This report covers the period from 1 July 2012 at 0800 to 1 October 2012 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/3Q12.php

2 Executive Summary

- XE6 utilisation in 3Q12 was 67%. Further details are available in Section 3.2 of the report.

- The system was again very reliable. There were 2 service failures in 3Q12 as opposed to 3 in 2Q12. There was one maintenance overrun and one job scheduling issue. The overall MTBF improved on 2Q12 from 732 hours to 1098 hours.

- The volume of single node failures remained low.

- Usage of the Research Data facility (RDF) continues to grow slowly. The RDF comprises of 7.8PB of disk storage, of which 114TB is now in use. Further work is still required to enhance the mechanisms in place for transferring data to/from the RDF to HECToR, the NERC LMS and external sites.

- New queues supporting 24 hour jobs were introduced on 4th July. These will be available for an initial 6 month trial period. These jobs accounted for approximately 14% of the overall utilization during this quarter.

- The PRACE allocations on HECToR appear to be working well. PRACE has a maximum 5% allocation on the service, and in 3Q12 the PRACE utilisation rose to 4.6%. The original batch of PRACE projects have now ended, but further projects will be allocated HECToR resource with each DECI call (two per year). The next batch of projects will commence in November.

3 Quantitative Metrics

3.1 Reliability

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

	Jul	Aug	Sep
Incidents	21	12	10
Failures	2	0	0

3.1.1 Performance Statistics
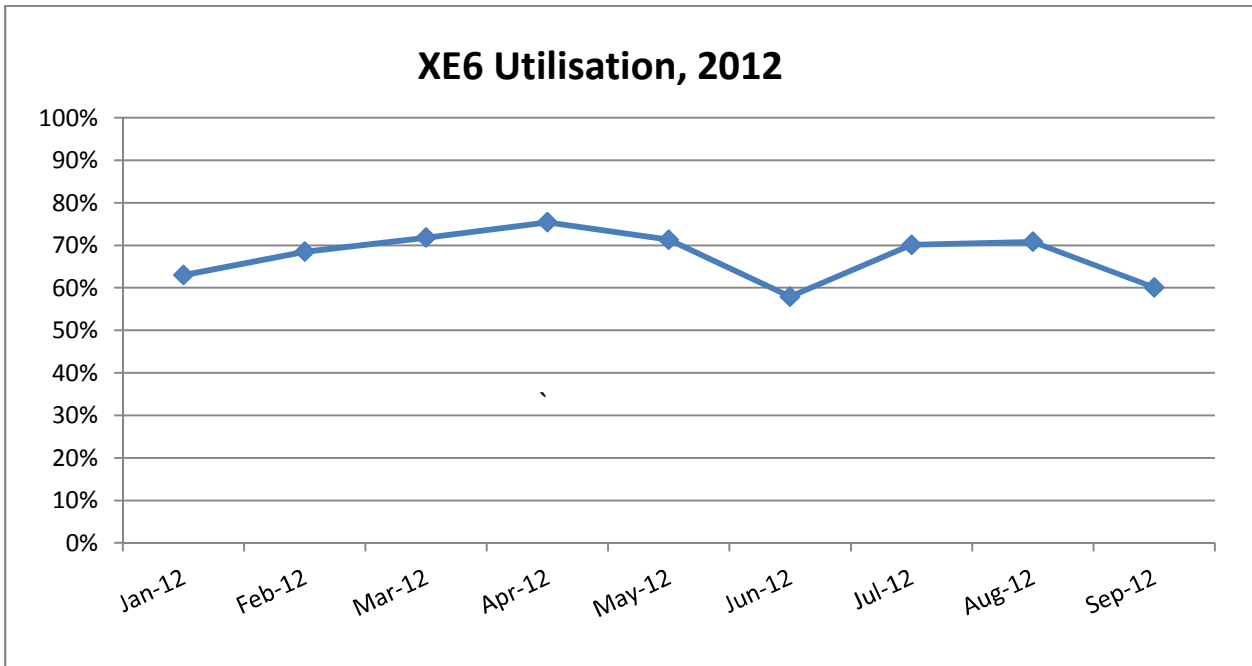
MTBF = (732)/(number of failures in a month)

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

Attribution	Metric	Jul	Aug	Sep	Quarterly
Technology	Failures	2	0	0	2
	MTBF	366	∞	∞	1098
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	2	0	0	2
	MTBF	366	∞	∞	1098

3.2 HECToR Utilisation

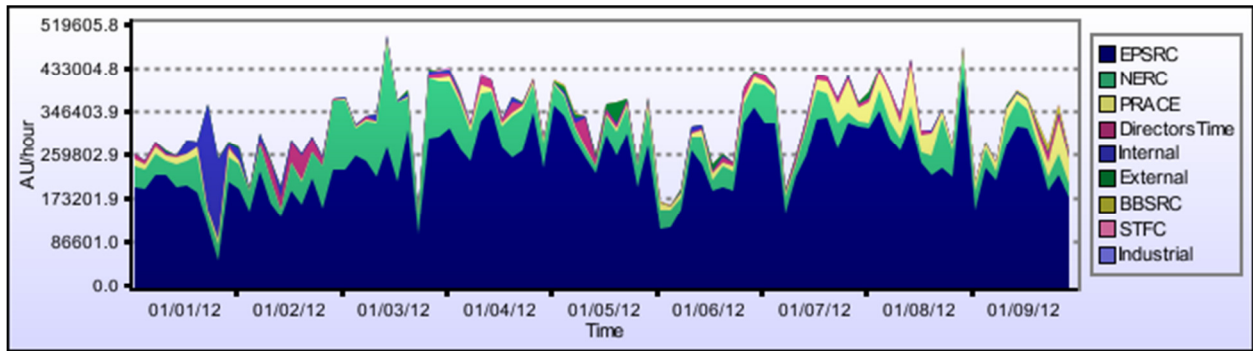## 3.2.1 XE6 Utilisation

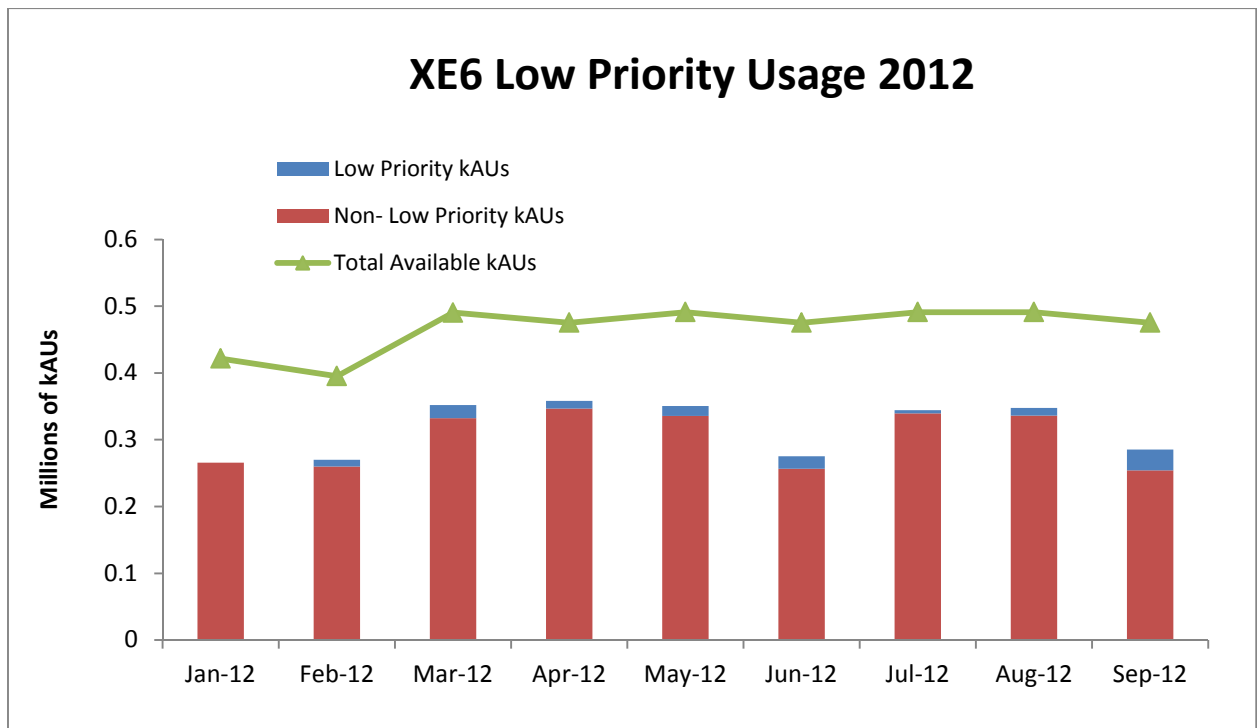The XE6 utilisation quarterly average in 3Q12 was 67.1%, compared to 68.2% in 2Q12.
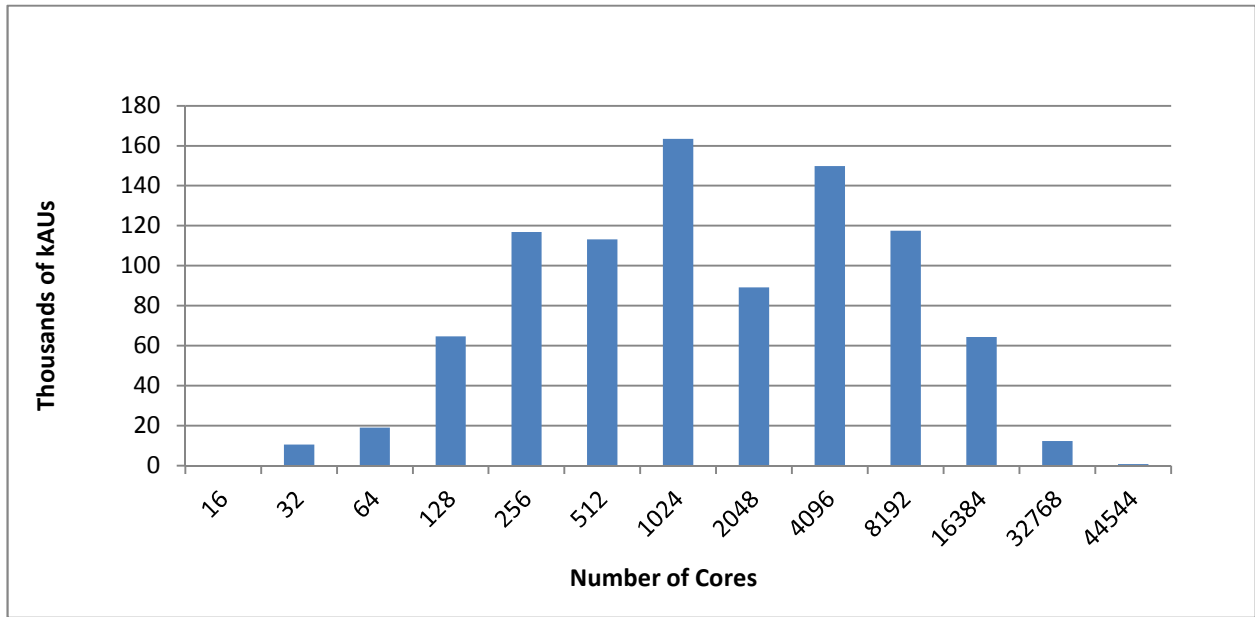
Capability Usage

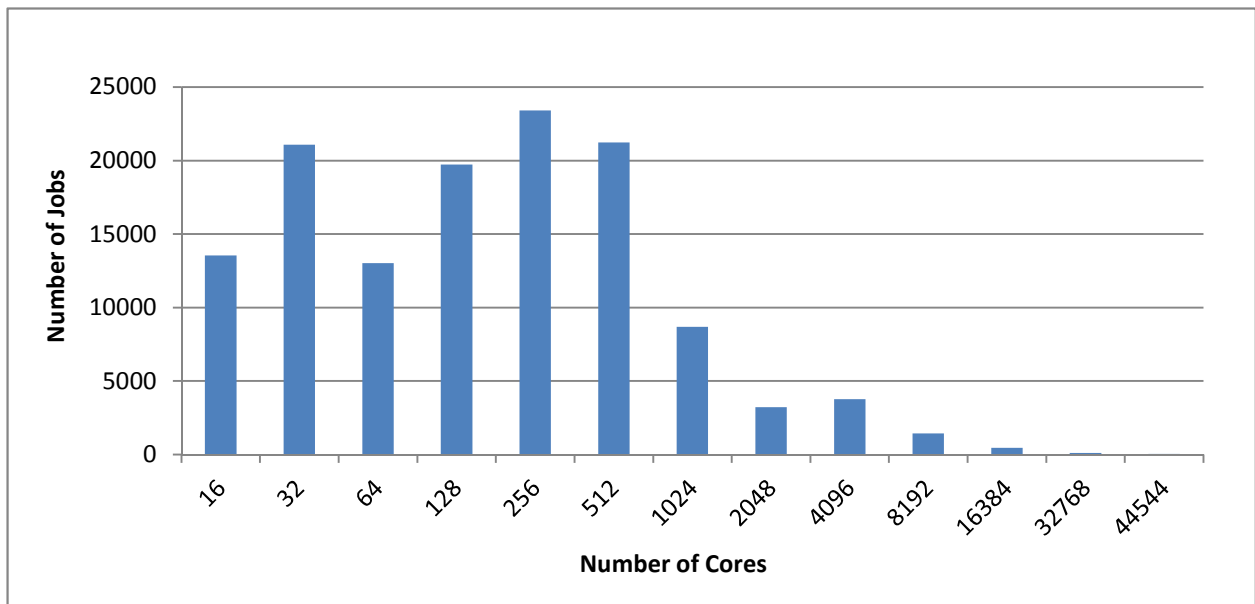**Raw AUs use by Funding Body of jobs using more than 511 CPUs**

Low Priority Access

In 3Q12, low priority access accounted for 5.14% the overall utilisation.

XE6 Low Priority Usage 2012

3.2.2 Utilisation by Core Count

3.2.3 Number of Jobs by Core Count

3.2.4 Utilisation by Consortium

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
y01	0.0	0.0	1	0.0%
y02	0.0	0.0	4	0.0%
y03	127.7	157.6	198	0.0%
y07	0.1	0.2	56	0.0%
z01	47.9	88.9	346	0.0%
z02	50.2	93.8	7	0.0%
z03	836.7	1482.4	994	0.1%
z12	16.9	20.4	10	0.0%
Internal Total	**1079.5**	**1843.4**	**1616**	**0.1%**
c01	7383.5	13830.6	2557	1.0%
e01	27497.0	66709.9	3887	4.6%
e05	167179.9	305986.6	36060	21.0%
e10	6019.9	10925.3	4343	0.8%
e24	5.4	10.1	21	0.0%
e71	289.0	539.0	84	0.0%
e76	899.6	1675.6	44	0.1%
e82	713.3	1226.9	96	0.1%
e89	16448.4	43435.5	5081	3.0%
e104	742.9	1353.1	593	0.1%
e106	3430.5	6313.7	560	0.4%
e107	0.7	1.3	318	0.0%
e108	13850.5	25060.6	210	1.7%
e110	12664.9	24783.1	741	1.7%
e122	4599.0	8460.3	1926	0.6%
e124	7201.1	21627.5	1187	1.5%
e125	6062.0	11143.5	196	0.8%
e126	3219.0	6016.7	94	0.4%
e127	1109.3	2013.6	118	0.1%
e128	2922.3	5288.9	219	0.4%
e129	917.3	1700.9	74	0.1%
e130	401.5	741.0	121	0.1%
e141	2610.2	4777.6	575	0.3%
e145	68.9	121.3	74	0.0%
e149	2323.4	4342.6	169	0.3%
e156	188.0	340.1	206	0.0%
e158	27.4	51.2	25	0.0%
e159	11.2	20.6	143	0.0%
e160	6347.4	11707.5	389	0.8%
e163	1589.0	2947.7	668	0.2%
e173	859.6	1592.7	391	0.1%
e174	2432.4	4477.3	86	0.3%
e175	3598.6	13899.2	476	1.0%
e177	213.5	399.0	158	0.0%
e179	481.0	887.4	70	0.1%
e185	32.8	57.0	23	0.0%
e186	8926.5	15526.6	826	1.1%
e187	25.8	46.3	181	0.0%
e192	775.6	1337.8	140	0.1%
e193	0.0	0.0	1	0.0%
e202	0.0	0.0	1	0.0%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
e203	443.0	790.6	196	0.1%
e204	402.1	742.3	50	0.1%
e207	25133.7	45918.3	112	3.2%
e212	0.0	0.0	2	0.0%
e213	8.0	13.7	42	0.0%
e220	0.0	0.0	12	0.0%
e224	0.0	0.0	2	0.0%
e228	7.8	14.5	4	0.0%
e229	958.8	1731.0	97	0.1%
e230	356.4	617.3	118	0.0%
e231	498.5	931.7	226	0.1%
e232	0.0	0.0	1	0.0%
e233	59.9	112.0	23	0.0%
e235	223.8	406.2	227	0.0%
e236	721.8	1349.1	861	0.1%
e240	133.4	245.1	113	0.0%
e244	6.7	11.9	233	0.0%
e245	221.9	398.1	342	0.0%
e246	0.0	0.0	1	0.0%
e247	0.0	0.0	1	0.0%
e248	120.7	206.7	54	0.0%
e249	1608.1	2930.1	207	0.2%
e250	1470.6	2590.6	36	0.2%
e251	5480.2	10234.3	57	0.7%
e252	4053.0	7291.5	349	0.5%
e253	3911.0	6804.3	284	0.5%
e256	37.9	64.8	72	0.0%
e258	97.2	181.7	13	0.0%
e260	977.9	1674.1	109	0.1%
e261	0.3	0.5	17	0.0%
e262	0.9	1.5	30	0.0%
e263	112.4	192.4	48	0.0%
e264	0.0	0.0	2	0.0%
j01	440.3	822.9	424	0.1%
EPSRC Total	**361554.2**	**707652.7**	**67497**	**48.5%**
n01	10279.4	18476.3	3707	1.3%
n02	34368.8	62065.5	23623	4.3%
n03	35949.4	66125.6	7048	4.5%
n04	6312.0	11662.9	10300	0.8%
NERC Total	**86909.5**	**158330.3**	**44678**	**10.9%**
b09	0.0	0.0	15	0.0%
b14	3473.0	6005.0	843	0.4%
b100	4.0	7.5	13	0.0%
BBSRC Total	**3477.0**	**6012.5**	**871**	**0.4%**
p01	209.1	390.5	55	0.0%
STFC Total	**209.1**	**390.5**	**55**	**0.0%**
e168	124.4	232.6	58	0.0%
x01	4929.8	9034.5	3204	0.6%
External Total	**5054.2**	**9267.0**	**3262**	**0.6%**
d03	0.0	0.0	3	0.0%
d04	0.9	1.7	2	0.0%
d11	2.9	5.2	84	0.0%
d15	1.6	2.7	91	0.0%

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
d25	2879.4	5309.0	962	0.4%
d26	108.4	135.1	168	0.0%
d27	9.4	17.1	186	0.0%
d29	15.7	28.0	61	0.0%
d32	87.5	160.5	328	0.0%
d34	102.0	190.7	1511	0.0%
d37	4266.6	8335.5	916	0.6%
d38	111.5	208.4	84	0.0%
d39	46.0	86.1	71	0.0%
d40	57.3	104.7	48	0.0%
d41	7258.4	13179.4	4288	0.9%
d45	0.0	0.0	40	0.0%
d46	0.2	0.4	8	0.0%
gd11	0.0	0.0	37	0.0%
DirectorsTime Total	**14947.8**	**27764.4**	**8888**	**1.9%**
pr1u0704	2275.2	3985.9	446	0.3%
pr1u0705	6813.8	12285.3	258	0.8%
pr1u0804	10129.9	18441.5	2069	1.3%
pr1u0805	2820.5	4828.4	162	0.3%
pr1u0807	0.0	0.0	11	0.0%
pr1u0808	13188.6	24650.8	45	1.7%
pr1u0809	1336.4	2296.4	30	0.2%
PRACE Total	**36564.3**	**66488.2**	**3021**	**4.6%**
x10	0.0	0.0	3	0.0%
x11	2.8	5.2	13	0.0%
Industrial Total	**2.8**	**5.2**	**16**	**0.0%**
Total	**509798.5**	**977754.2**	**129904**	**67.1%**

3.3 Helpdesk

A total of 1042 queries with a specified service metric and *147 queries with no metric were completed in this period.

*Setup tickets for the RDF have no metric associated as the RDF support is on a reasonable endeavours basis only. These tickets are not included in the summary below.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	831	857	97.0%	97.0%
Admin queries finished in 1 day	778	803	96.9%	97.0%
Queries assigned in 30 min	1024	1029	99.5%	97.0%
Technical assessments in 10 days	37	37	100.0%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	505	48.9%

Admin	298	28.9%
In-depth	138	13.4%
Technical	54	5.2%
Technical assessment class-1a	37	3.6%

Queries by Category

Query Category	Queries	Percentage
New User	156	13.2%
New Password	135	11.5%
Create Directory	94	8.0%
Access to HECToR	94	8.0%
None	86	7.3%
Set group quotas	64	5.4%
User behaviour	52	4.4%
3rd Party Software	51	4.3%
Set user quotas	50	4.2%
Batch system and queues	49	4.2%
Disk, tapes, resources	44	3.7%
Compilers and system software	44	3.7%
Make Reservation	38	3.2%
Login, passwords and ssh	35	3.0%
Other	29	2.5%
User programs	28	2.4%
Join Project	27	2.3%
New Group	20	1.7%
Courses	13	1.1%
Node Failure	11	0.9%
SAFE	10	0.8%
Create certificate	10	0.8%
Add to group	10	0.8%
gpu	8	0.7%
Remove account	6	0.5%
Static website	5	0.4%
Grid	4	0.3%
Update account	2	0.2%
Performance and scaling	2	0.2%
Delete from project	1	0.1%
Archive	1	0.1%

Queries by Handler Category

Handlers	Technical	In-depth	Admin	TA	Automatic	Total	%age
OSG	11	8	28		505	552	53.5%
USL	36	46	266			348	33.7%
CSE	1	60		37		98	9.5%
Cray	6	24	4			34	3.3%

3.3.1 Quality Tokens

Five positive quality tokens were received in 3Q12. There were no negative tokens.

Project	Positive Tokens	Negative Tokens
e05	5	0
Total	**5**	**0**

3.4   Performance Metrics

Metric	TSL(%)	FSL(%)	Jul-12	Aug-12	Sep-12	3Q12
Technology Reliability (%)	85.00%	98.50%	99.6	100.0	100.0	99.9%
Technology MTBF (hours)	100	126.4	366.0	∞	∞	732
Technology Throughput, hours/year	7000	8367	8637.8	8654.4	8646.0	8646.1
Capability jobs completion rate	70%	90%	100.0%	100.0%	95.5%	98.5%
Non in-depth queries resolved within 1 day (%)	85%	97%	99.3%	97.3%	95.0%	97.0%
Number of SP FTEs	7.3	8.0	7.8	9.1	8.4	8.4
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

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	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
EPSRC Projects							
c01	Support of EPSRC/STFC SLA	EPSRC	Class1a	Dr Adrian Wander	54,803.70	51,483.30	3,320.40
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	483,969.90	151,123.80	332,708.80
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1,139,124.00	818,519.70	319,928.80
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257,748.20	22,453.00	235,295.20
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50,000.00	49,887.50	112.5
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130,403.50	54,729.20	75,662.70
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42,521.80	40,897.90	1,623.90
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	4,853.40	2,833.50	2,019.80
e84	Vortical Mode Interactions	EPSRC	Class1a	Dr Tamer Zaki	9,600.00	3,203.10	6,396.90
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8,088.60	6,285.60	1,803.00
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	400,100.00	358,404.80	41,695.20
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30,400.00	10,317.70	20,078.50
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1a	Dr Andreas M Kempf	1,300.00	297.3	1,002.70
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1a	Prof Kai Luo	3,650.00	3,430.80	219.2

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e107	Parallel Brain Surgery Simulation	EPSRC	Class1a	Dr Stephane P. A. Bordas	6,000.00	721.6	5,278.40
e108	Jet Flap Noise	EPSRC	Class1a	Dr Sergey Karabasov	49,684.50	45,068.20	4,616.20
e110	Computational Aeroacoustics Consortium	EPSRC	Class1a	Prof Paul Tucker	140,110.30	91,812.30	48,236.10
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	150,000.00	75,299.80	74,700.20
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Prof Richard D Sandberg	22,887.90	23,224.20	-344.3
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168,324.80	37,544.50	130,670.40
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25,584.00	17,313.40	8,270.60
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7,000.00	3,290.40	3,709.60
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7,092.10	6,691.80	400.4
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7,500.00	2,627.10	4,872.90
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10,500.00	4,742.40	5,757.60
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16,350.00	7,184.50	9,165.50
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1,191.90	473.2	716.2
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68,082.50	50,802.60	17,279.90
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10,000.00	161.7	9,838.30
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1,600.00	331.6	1,268.40
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	2,500.00	439	2,061.00

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3,816.00	35.7	3,780.30
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20,208.10	15,407.80	4,800.30
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69,895.50	0	69,895.50
e163	Numerical Simulation of Spontaneous Ignition	EPSRC	Class1b	Prof Jennifer Wen	4,142.30	2,704.80	1,437.50
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4,872.00	0	4,872.00
e173	Performance of oomph-lib in largescale parallel computations	EPSRC	Class1b	Prof Matthias Heil	4,800.00	1,626.00	3,174.00
e174	3D instabilities in two-layer flows	EPSRC	Class1b	Dr Prashant Valluri	11,495.40	3,598.90	7,896.50
e175	Fine-Scale Turbulence	EPSRC	Class1a	Prof Richard D Sandberg	50,000.00	5,944.00	43,900.30
e177	Amorphous structures of mirror coatings	EPSRC	Class1b	Dr Ian Maclaren	5,700.80	3,125.60	2,575.10
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87,000.00	2,873.30	84,126.70
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8,150.20	0	8,150.20
e183	Analysis of Processes in Hydrocarbon Fuel Droplets	EPSRC	Class1a	Prof Sergei Sazhin	8,640.00	69.7	8,570.30
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130,500.00	1,387.10	129,112.90
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340,000.00	6,175.50	333,824.50
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70,000.00	58,334.20	11,665.80
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6,030.20	647.3	5,382.80
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40,500.00	4,413.10	36,086.90

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e192	Physical properties of carbon nanotubes	EPSRC	Class1b	Dr Michael R C Hunt	10,963.00	5,421.80	5,541.10
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38,345.00	5,072.50	33,272.50
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim Biktashev	4,499.60	2,222.50	2,277.10
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5,000.00	412.5	4,587.50
e206	FLAME Agent-Based Simulation Framework	EPSRC	Class1a	Prof Christopher Greenough	410	0	410
e207	Developing DL_POLY Molecular Dynamics Simulation code	EPSRC	Class1a	Dr Kostya Trachenko	25,857.60	18,040.40	7,817.20
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	8.3	391.7
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26,121.60	17,021.60	9,100.00
e223	Numerical modelling of aorta dissection	EPSRC	Class2a	Prof. Xiaoyu Luo	300	0	300
e226	Novel Vibrational Spectroscopic Techniques	EPSRC	Class1a	Dr Andrew D Burnett	1,032.30	0	1,032.30
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50	46.4	3.6
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	20,218.30	353.7	19,864.60
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50,000.00	8,969.20	41,030.80
e230	Adsorption and Diffusion in Metal-Organic Frameworks	EPSRC	Class2a	Dr Ahmet Ozgur Yazaydin	918.9	877.5	41.4
e231	Rapid Alloy Solidification	EPSRC	Class1b	Prof Peter Jimack	5,130.00	773.4	4,356.60
e235	Modelling offshore wind	EPSRC	Class2a	Prof Simon Watson	400	400.5	-0.5
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400	399	1

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e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	307.5	492.5
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	1.4	498.6
e242	Study of the Green Fluorescent Protein Fluorophore	EPSRC	Class2a	Dr Garth Jones	400	0	400
e243	Tailored Structures for Orthopaedic Implantations	EPSRC	Class2a	Dr Carmen Torres-Sanchez	400	0	400
e244	VOX-FE: Large Scale FE Bone Modelling on HECToR	EPSRC	Class2b	Prof Michael Fagan	800	8.4	791.6
e245	Parallelisation of a harmonic balance NS solver	EPSRC	Class2b	Dr Sergio Campobasso	800	631.2	168.8
e246	Numerical simulation of capillary blood flow	EPSRC	Class2a	Dr Ellak Somfai	400	0	400
e247	Tool development for multiscale protein folding simulations	EPSRC	Class2a	Dr Robert Best	400	220.9	179.1
e248	Testing of a Distributed Coordinate Descent Method	EPSRC	Class2a	Dr Peter Richtarik	400	102.4	297.6
e249	Feedback flow control for reducing the aerodynamic drag	EPSRC	Class1b	Dr Aimee Morgans	9,860.00	2,370.90	7,489.10
e250	Thermal Mixing around In-line Tube Banks	EPSRC	Class1b	Prof Hector Iacovides	2,002.00	1,635.90	366.1
e251	Asynchronous Genetic Algorithms in HPC Gait Simulation	EPSRC	Class1b	Dr Bill Sellers	13,200.00	8,963.50	4,236.50
e252	LES of flows around wind turbine blades	EPSRC	Class1b	Dr Zheng-Tong Xie	7,740.00	7,697.10	42.9
e253	Turbulent premixed and stratified combustion	EPSRC	Class1b	Prof Stewart Cant	14,221.00	14,994.60	-773.6
e254	Ceramic Composites for Fusion Power	EPSRC	Class1b	Prof Sergei Dudarev	8,371.00	0	8,371.00
e255	Turbulent Drag Reduction	EPSRC	Class2a	Dr Pierre Ricco	400	0	400
e256	Hybrid simulation on heat transfer	EPSRC	Class2a	Dr Huasheng Wang	300	37.9	262.1

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e257	Global stability and sensitivity of fuel injectors	EPSRC	Class1b	Dr. Matthew P Juniper	1,728.00	28.1	1,699.90
e258	Morphology and electronic props of semiconducting polymers	EPSRC	Class1b	Prof Alessandro Troisi	5,650.00	729.2	4,920.80
e259	DNS of multi-species fuel combustion	EPSRC	Class1b	Dr N Swaminathan	31,505.00	2,101.40	29,403.60
e260	Microscopic gas diffusion-reaction model	EPSRC	Class1a	Dr Jochen Blumberger	4,940.00	1,502.20	3,437.80
e261	Expressive and scalable finite element simulation	EPSRC	Class2b	Dr Garth Wells	800	0.3	799.7
e262	MC simulations of semiconductor nanostructures	EPSRC	Class2a	Prof Ian Galbraith	300	0.9	299.1
e263	Modelling the Elastic and Moisture Barrier Properties of Skin	EPSRC	Class2a	Dr Rebecca Notman	300	235.8	64.2
e264	Metabolic efficiency in neurons with extended morphology	EPSRC	Class2a	Dr Biswa Sengupta	300	0.1	299.9
e265	HPC for the Discrete Element Method User Community	EPSRC	Class2b	Dr Catherine O'Sullivan	800	0	800
e266	Thermal and Reactive Flow Simulation on High-End Computers	EPSRC	Class1a	Prof Kai Luo	226,800.00	0	226,800.00
STFC Projects							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	10,002.70	2,987.00	7,015.70
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	220,690.90	180,854.00	39,836.90
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	dr grenville gms lister	676,027.50	495,909.10	180,118.40
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	538,860.70	449,207.70	89,653.00
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	152,305.70	108,703.20	43,602.50

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n99	NERC Training	NERC	Class1a	dr grenville gms lister	2	0	2
BBSRC Projects							
b09	Circadian Clock	BBSRC	Class1a	Materials	Prof Andrew A Millar	2,000.00	1,394.40
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Life Sciences	Dr Michael Ball	10,000.00	639.9
b12	Flu Analysis on HECToR	BBSRC	Class1a	Life Sciences	Mr Adrian Jackson	50	0
b13	Linear Scaling DFT for Biochemistry Applications	BBSRC	Class1a	Physics	Dr David Bowler	5,587.20	105.6
b14	Understanding supercoiling-dependent DNA recognition	BBSRC	Class1a	Life Sciences	Prof Anthony Maxwell	42,600.00	11,434.80
Director's Time							
d04	MSc in HPC	DirectorsTime	Service	Dr David Henty	613.5	478.1	135.4
d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	10,000.00	5,009.10	4,990.90
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	102	14.5	87.5
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1,000.00	18.6	981.4
d23	TEXT FP7	DirectorsTime	Service	Dr Mark Bull	1,500.00	35.6	1,464.40
d24	SBSI	DirectorsTime	Service	Dr Stephen Gilmore	2,000.00	958.1	1,041.90
d25	Code Scaling	DirectorsTime	Service	Dr Ken Rice	51,500.00	11,877.40	39,622.60
d26	Guest Training Accounts	DirectorsTime	Service	Miss Elizabeth Sim	550	478.2	71.8
d27	RR	DirectorsTime	Service	Mr Paul Graham	100	64.7	35.3

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d29	Nu-FuSe	DirectorsTime	Service	Mr Adrian Jackson	1,500.00	404	1,096.00
d30	PARTRAC	DirectorsTime	Service	Dr Mark Sawyer	200	124	76
d32	APOS-EU	DirectorsTime	Service	Dr Michele Weiland	1,000.00	283.7	716.3
d34	Msc 2011-2012	DirectorsTime	Service	Dr David Henty	1,000.00	189.6	810.4
d35	PhD	DirectorsTime	Service	Dr Mark Bull	10	0	10
d36	Genome	DirectorsTime	Service	Dr Alan Gray	3,460.00	0	3,460.00
d37	CRESTA	DirectorsTime	Service	Dr Lorna Smith	21,000.00	7,622.70	13,377.30
d38	Windfarm Simulation	DirectorsTime	Service	Mr Adrian Jackson	471	410.1	60.9
d39	NCSA access	DirectorsTime	Service	Mr Mark A Straka	1,000.00	986.1	13.9
d40	Computational Chemistry at St Andrews	DirectorsTime	Service	Dr Herbert Fruchtl	2,000.00	204.9	1,795.10
d41	NPL Project	DirectorsTime	Service	Dr Ulrich Zachariae	45,000.00	26,448.90	18,551.10
d42	Oxford Nanopore Technologies	DirectorsTime	Service	Dr Jayne Wallace	1,170.20	734.2	436
d43	IS Apps	DirectorsTime	Class2b	Mr Tony Weir	13,000.00	0	13,000.00
d44	Crucible	DirectorsTime	Service	Mr Iain A Bethune	1,000.00	0	1,000.00
d45	MSc in HPC 2012-2013	DirectorsTime	Service	Dr David Henty	1,000.00	28.4	971.6
d46	Silicate melts with CP2K	DirectorsTime	Service	Mr Iain A Bethune	500	0.2	499.8
d47	PGS Project	DirectorsTime	Service	Dr Kevin Stratford	100	0	100

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gd01	testing the GPU	DirectorsTime	Service	Dr Murray Cole	0	0	0
gd04	MSC in HPC - GPU Research	DirectorsTime	Service	Dr David Henty	0	0	0
gd05	Musical Acoustics (PhD Project)	DirectorsTime	Service	Dr Alan Gray	0	0	0
External Projects							
e168	TEXT	External	Service	Dr Mark Bull	1,500.00	79.5	1,420.50
x01	HPC-Europa	External	Service	Dr Judy Hardy	41,762.40	34,954.70	6,807.70
x02	BlueArc (TDS)	External	Service	Mr M W Brown	1	0	1
PRACE Projects							
pr1u0000	Generic PRACE	PRACE	Service	Dr Chris A Johnson	0	0	0
pr1u0001	PRACE Staff	PRACE	Class1a	Miss Elizabeth Sim	1	0	1
pr1u0701	EC4aPDEs-2	PRACE	Class1a	Dr Chris A Johnson	0	0	0
pr1u0702	HYDROGEN-ILs	PRACE	Class1a	Dr Chris A Johnson	0	0	0
pr1u0703	HELIXKINETICS	PRACE	Class1a	Dr Chris A Johnson	0	0	0
pr1u0704	HIFLY	PRACE	Class1a	Dr Chris A Johnson	8,450.40	6,339.70	2,110.70
pr1u0705	TanGrin	PRACE	Class1a	Dr Chris A Johnson	14,084.00	14,042.10	41.9
pr1u0706	SIVE-2	PRACE	Class1a	Dr Chris A Johnson	14,000.00	5,376.90	8,623.10
pr1u0801	CONTRAR	PRACE	Class1a	Dr Chris A Johnson	1	0	1

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pr1u0802	POLARIZABLEFOLDBIND	PRACE	Class1a	Dr Chris A Johnson	1	0	1
pr1u0803	TLRSim	PRACE	Class1a	Dr Chris A Johnson	1	0	1
pr1u0804	FULLDRUG	PRACE	Class1a	Dr Chris A Johnson	14,874.00	15,003.40	-129.4
pr1u0805	NanoTherm	PRACE	Class1a	Dr Chris A Johnson	7,669.80	7,725.30	-55.5
pr1u0806	NELC	PRACE	Class1a	Dr Chris A Johnson	11,408.00	0	11,408.00
pr1u0807	PARAMETER	PRACE	Class1a	Dr Chris A Johnson	6,720.00	1.2	6,718.80
pr1u0808	PIPETURB	PRACE	Class1a	Dr Chris A Johnson	12,600.00	11,109.40	1,490.60
pr1u0809	VIPforVPH	PRACE	Class1a	Dr Chris A Johnson	5,346.00	1,161.90	4,184.10
pr1u0810	DrugEffluxMechanism	PRACE	Class1a	Dr Chris A Johnson	4,964.80	0	4,964.80
pr1u9999	PRACE Training	PRACE	Class1a	Dr David Henty	0	0	0