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HECToR Quarterly Report

Apr 2013 – Jul 2013

1 Introduction

This report covers the period from 1 April 2013 at 0800 to 1 July 2013 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/2Q13.php

2 Executive Summary

- XE6 utilisation in 2Q13 was 86.8% compared to 79.9% in 1Q13. This equates to 108.5% of the optimum 80%. Despite the sustained period of increased utilisation on the service, there have been no reports from users of this having affected their research throughput. The UK Materials Chemistry Consortium (e05) accounted for over 25% of the total utilisation. Further details are available in Section 3.2 of the report.

- There were three service failures in 2Q13. There was one batch scheduler failure, and one cabinet power supply failure. The third failure was as a result of a fault on a management server which caused the network to hang. The overall MTBF was 732 hours.

- Downtime due to scheduled maintenance was kept to a minimum in 2Q13, with less than 10 hours scheduled downtime in total. The concept of using 'at-risk' periods for non-intrusive maintenance has worked well.

- The volume of single node failures remained low.

- The 24-hour queues have been an integral part of the service since January. Jobs in these queues accounted for 16.6% of the utilisation in the quarter.

- Low priority jobs accounted for 1.6% of the utilisation in 2Q13. Further details are available in Section 3.2.

- The helpdesk statistics were excellent. The service targets were surpassed in all areas. Further details are in Section 3.

- The HECToR Archive is 80% full and is not expected to be sustained in ARCHER. A five step plan was agreed at the HECToR Scientific Advisory Committee meeting in May to copy the user data from the Archive to the UK Research Data Facility (RDF). As part of this plan the HECToR Archive was made read only in June and users have been encouraged to use the RDF instead. The Archive has also been directly connected to the RDF and testing is currently underway regarding the transfer of user data. An outline timetable will be communicated to users once the testing is complete.

- A user meeting to discuss the RDF is being held in London on 30th July. Representatives from the HECToR service and various user groups will be in attendance.

3 Quantitative Metrics

3.1 Reliability

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

	Apr	May	Jun
Incidents	14	12	14
Failures	1	0	2

3.1.1 Performance Statistics

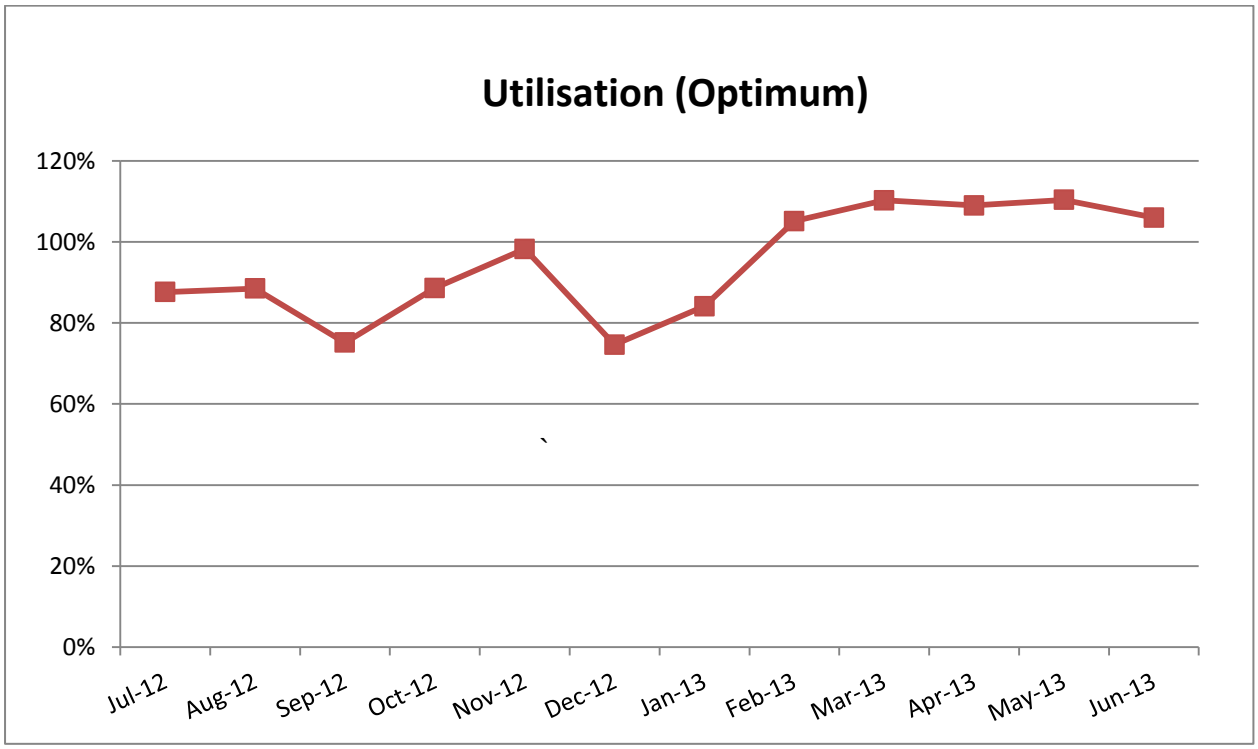
MTBF = (732)/(number of failures in a month)

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

Attribution	Metric	Apr	May	Jun	Quarterly
Technology	Failures	1	0	2	3
	MTBF	732	∞	366	732
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External/Other	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	1	0	2	3
	MTBF	732	∞	366	732

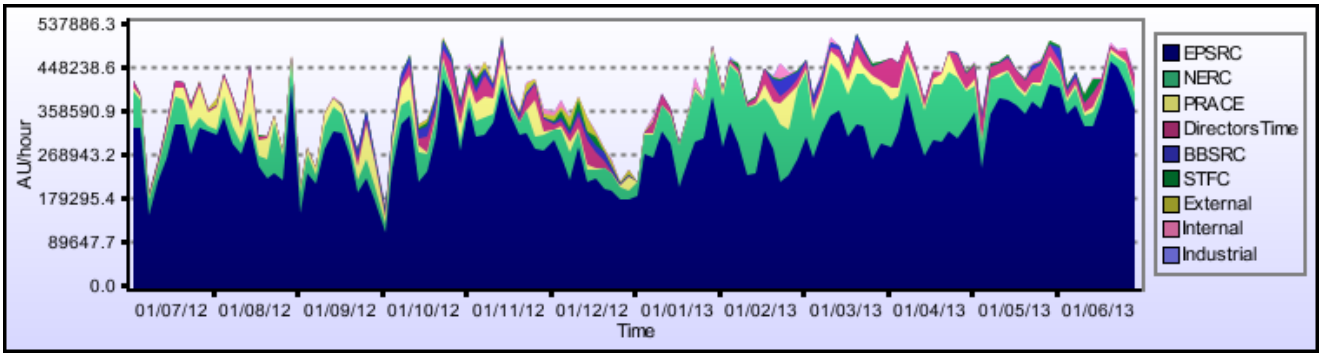
3.2 HECToR Utilisation

3.2.1 XE6 Utilisation



The XE6 utilisation quarterly average in 2Q13 was 108.5% of optimum, compared to 99.9% in 1Q13.

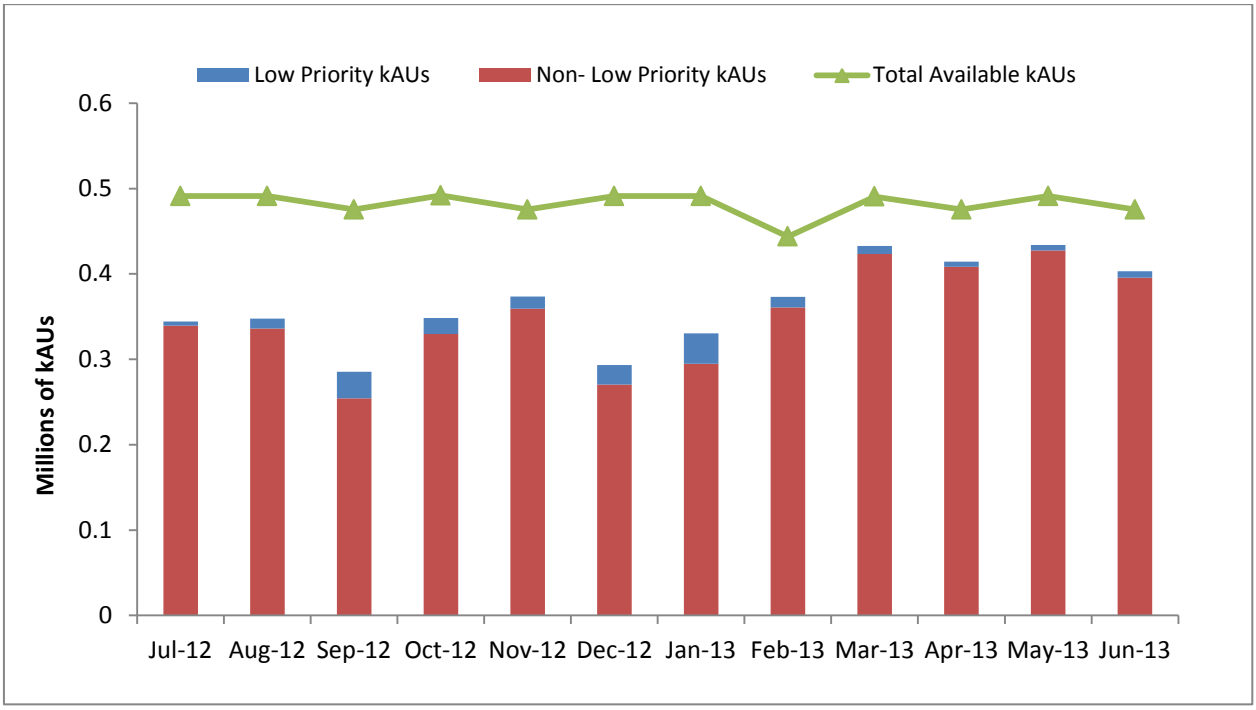
3.2.2 Capability Usage



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

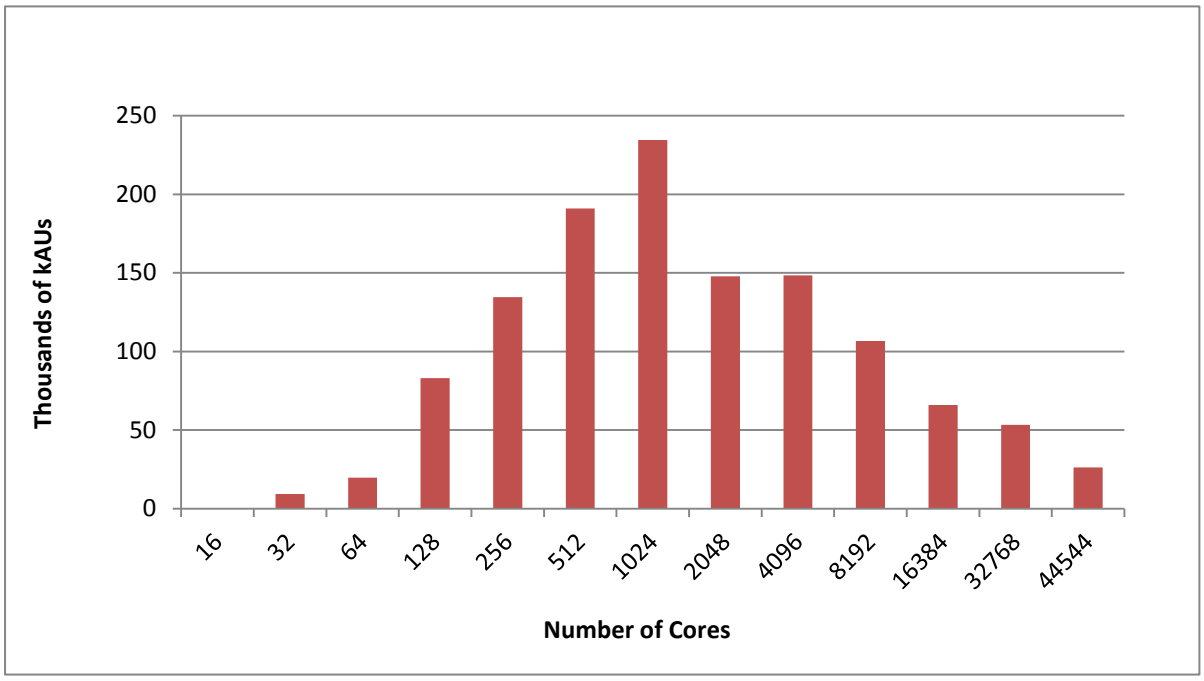
3.2.3 Low Priority Access

In 2Q13, low priority access accounted for 1.6% the overall utilisation.

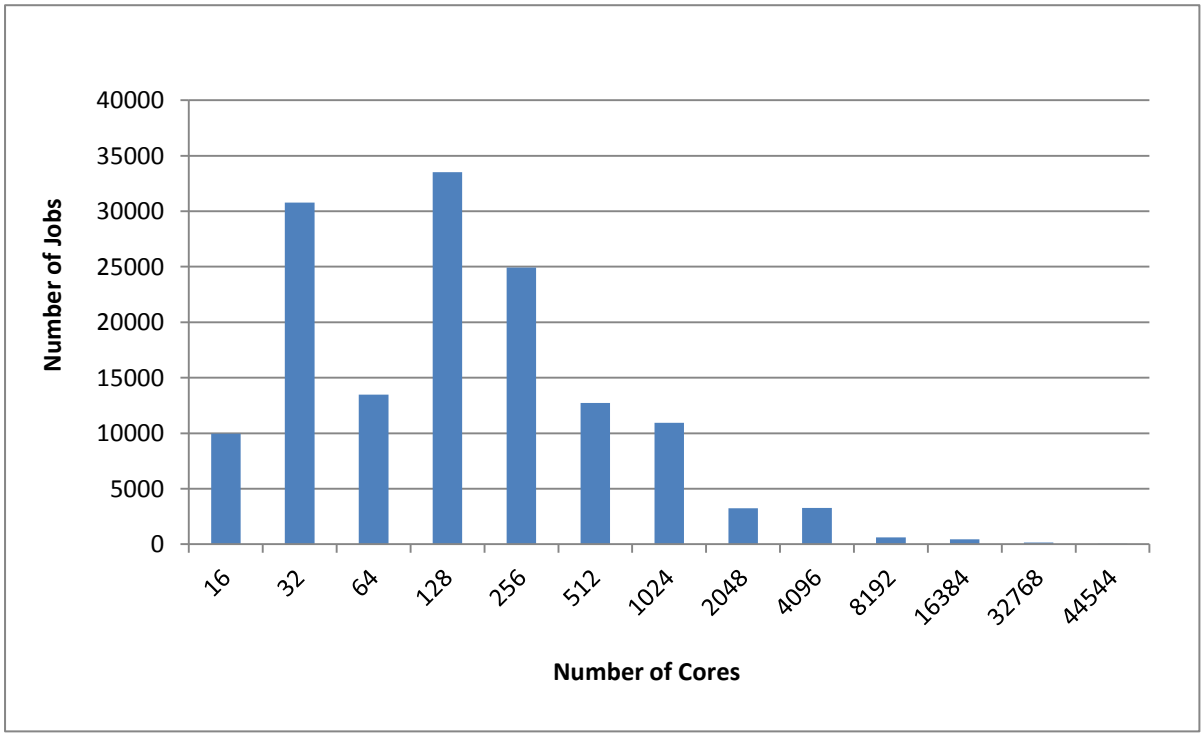


The low priority queues are only enabled when the paid backlog on the system is low, or in the run up to maintenance sessions. The utilisation of the service has been at such a level in 2Q13 that the low priority queues have rarely been enabled.

3.2.4 Utilisation by Core Count



3.2.5 Number of Jobs by Core Count



3.2.6 Utilisation by Consortium

Project	kAUs	Raw kAUs	Number of Jobs	Utilisation
y03	438	502	1604	0.03%
z01	380	657	4456	0.05%
z03	1153	2876	996	0.20%
Internal Total	2034	4107	7103	0.28%
c01	7244	12580	1748	0.87%
e01	36505	71474	4100	4.96%
e05	196576	363797	42221	25.23%
e10	4273	7534	1645	0.52%
e68	13	23	7	0.00%
e71	2913	4990	345	0.35%
e76	697	1209	154	0.08%
e82	8	13	107	0.00%
e89	45376	86100	10786	5.97%
e104	1210	2072	255	0.14%
e107	0	90	72	0.01%
e108	4094	7009	343	0.49%
e110	25214	43617	988	3.02%
e122	38283	65722	3324	4.56%
e125	1225	2144	304	0.15%
e126	3549	6076	32	0.42%
e141	383	655	131	0.05%
e145	317	542	425	0.04%
e149	449	774	83	0.05%
e155	335	573	71	0.04%
e156	71	122	153	0.01%
e158	286	561	87	0.04%
e159	101	173	464	0.01%
e160	2235	3826	362	0.27%
e174	490	840	105	0.06%
e175	3830	10468	648	0.73%
e179	1024	1753	127	0.12%
e182	536	917	88	0.06%
e184	942	1613	94	0.11%
e185	755	1292	51	0.09%
e186	19	33	9	0.00%
e187	49	84	190	0.01%
e202	10885	19210	392	1.33%
e203	134	230	152	0.02%
e204	944	1617	108	0.11%
e207	2488	7994	36	0.55%
e228	1353	2315	275	0.16%
e229	8444	14456	569	1.00%
e231	4027	6894	329	0.48%
e235	229	392	249	0.03%
e248	5	8	58	0.00%
e254	2142	5228	333	0.36%
e259	5266	15105	16	1.05%
e260	658	1126	295	0.08%
e262	5	8	42	0.00%
e263	22019	37721	1371	2.62%
e265	270	462	76	0.03%

e266	5112	8900	1167	0.62%
e269	4375	7733	279	0.54%
e270	9975	24629	152	1.71%
e271	18513	44973	364	3.12%
e272	11770	20150	490	1.40%
e273	145	248	75	0.02%
e274	149	256	71	0.02%
e275	23	39	33	0.00%
e276	24	41	18	0.00%
e278	110	190	17	0.01%
e279	75	128	40	0.01%
e281	3	6	3	0.00%
e282	5	9	91	0.00%
j01	425	1330	78	0.09%
EPSRC Total	**488579**	**920080**	**76756**	**63.81%**
n01	22021	37711	3763	2.62%
n02	36017	61665	26951	4.28%
n03	54847	93893	14024	6.51%
n04	15094	25892	5543	1.80%
NERC Total	**127978**	**219161**	**50281**	**15.20%**
b09	15	25	63	0.00%
b14	5315	9098	853	0.63%
b15	242	414	77	0.03%
b16	2720	4656	63	0.32%
BBSRC Total	**8291**	**14193**	**1056**	**0.98%**
p01	3822	6871	195	0.48%
STFC Total	**3822**	**6871**	**195**	**0.48%**
b10	5	8	169	0.00%
d11	317	547	152	0.04%
d15	105	266	229	0.02%
d25	546	934	251	0.06%
d26	560	682	1251	0.05%
d29	91	245	50	0.02%
d37	1623	4339	619	0.30%
d40	209	357	95	0.02%
d41	16386	28050	959	1.95%
d43	14046	24046	429	1.67%
d45	160	274	2099	0.02%
d49	1	1	10	0.00%
d51	36	62	30	0.00%
Directors Time Total	**34083**	**59812**	**6346**	**4.15%**
pr1u0002	162	343	244	0.02%
pr1u0806	3591	6147	91	0.43%
pr1u0807	2027	3890	322	0.27%
pr1u0902	2467	4224	104	0.29%
pr1u0903	779	1334	475	0.09%
pr1u0904	2569	4397	131	0.30%
pr1u0905	201	344	328	0.02%
pr1u0907	1436	2458	11	0.17%
pr1u1004	18	57	22	0.00%
pr1u1008	2123	3634	53	0.25%
pr1u1009	95	162	69	0.01%
pr1u1011	5	8	409	0.00%
pr1u1012	0	1	7	0.00%
PRACE Total	**15473**	**26998**	**2266**	**1.87%**

i02	6	10	24	0.00%
i03	6	10	34	0.00%
i04	102	175	92	0.01%
i06	39	66	29	0.00%
Industrial Total	**152**	**261**	**188**	**0.02%**
Total	**680413**	**1251483**	**144203**	**86.79%**

3.3 Helpdesk

A total of 1241 queries with a specified service metric, and 756 queries with no metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	1101	1121	98.2%	97.0%
Admin queries finished in 1 day	1063	1079	98.5%	97.0%
Queries assigned in 30 min	1235	1241	99.5%	97.0%
Technical assessments in 10 days	10	10	100.0%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	779	62.8%
Admin	300	24.2%
In-depth	110	8.9%
Technical	42	3.4%
Technical Assessment	10	0.8%

Queries by Category

Query Category	Queries	Percentage
Set group quotas	161	13.0%
New User	154	12.4%
Add to group	139	11.2%
New Password	121	9.8%
Set user quotas	78	6.3%
Disk, tapes, resources	61	4.9%
3rd Party Software	56	4.5%
Access to HECToR	53	4.3%
New Group	49	3.9%
None	48	3.9%
User behaviour	42	3.4%
Compilers and system software	37	3.0%
User programs	32	2.6%
Batch system and queues	27	2.2%
Login, passwords and ssh	24	1.9%
Make Reservation	21	1.7%
Other	20	1.6%
Join Project	20	1.6%
Create certificate	19	1.5%
Courses	19	1.5%
Node Failure	16	1.3%

SAFE	15	1.2%
Update account	14	1.1%
Archive	4	0.3%
Performance and scaling	3	0.2%
Grid	3	0.2%
gpu	1	0.1%
Remove account	1	0.1%
Network	1	0.1%
Delete from group	1	0.1%
Delete Certificate	1	0.1%

Queries by Handler Category

Handlers	Admin	Technical	Technical Assessment	Automatic	In-depth	Total	%age
USL	261	31			36	328	26.4%
CSE			10		59	69	5.6%
OSG	33	8		779	2	822	66.2%
Cray	6	3			13	22	1.8%

3.3.1 Quality Tokens

There were no tokens set in 2Q13.

3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Apr-13	May-13	Jun-13	2Q13
Technology Reliability (%)	85.0%	98.5%	97.9%	100.0%	98.1%	98.7%
Technology MTBF (hours)	100	126.4	732	∞	366	732
Technology Throughput, hours/year	7000	8367	8603	8724	8565	8630
Capability jobs completion rate	70.0%	90.0%	100.0%	100.0%	100.0%	100.0%
Non in-depth queries resolved within 1 day (%)	85.0%	97.0%	98.1%	98.5%	98.1%	98.2%
Number of SP FTEs	7.3	8.0	8.3	9.3	9.7	9.1
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	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	113303	61480	51823
e01	UK Turbulence Consortium	EPSRC	Class1a	Prof Richard D Sandberg	2319369	233122	2086248
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	6319874	1338872	4980942
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257748	35033	222572
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1a	Dr Nicolas Smiths	30400	14171	16225
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50000	49901	99
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130404	68401	61991
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42522	42267	255
e85	Study of Interacting Turbulent Flames	EPSRC	Class1a	Dr N Swaminathan	8089	6286	1803
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1a	Dr Matt Probert	2403145	453910	1949235
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	150000	140757	9243
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168325	42613	125601

e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25584	24754	830
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7000	4419	2581
e128	Rate-Controlled Constrained Equilibrium	EPSRC	Class1a	Dr Stelios Rigopoulos	7092	6692	400
e129	Novel Hybrid LES-RANS schemes [ICL]	EPSRC	Class1a	Prof Michael Leschziner	7500	2627	4873
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16350	8256	8094
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1192	846	344
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68083	56419	11663
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10000	1844	8157
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	2500	1136	1364
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3816	172	3644
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	40208	20012	20196
e161	Properties and Dynamics of Atomic Bose-Einstein Condensates	EPSRC	Class1a	Dr A White	69896	0	69896
e165	Multi-scale simulation of intense laser plasma interactions	EPSRC	Class1a	Dr Tony Arber	4872	0	4872
e174	3D instabilities in two-layer flows	EPSRC	Class1a	Dr Prashant Valluri	35495	4918	30577
e175	Fine-Scale Turbulence	EPSRC	Class1a	Prof Richard D Sandberg	50000	14943	34902

e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87000	4722	82278
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8150	618	7532
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130500	2741	127759
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340000	9021	330979
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70000	69785	215
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6030	1078	4952
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40500	4413	36087
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38345	35686	2659
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim N. Biktashev	5500	4356	1144
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5000	3867	1133
e206	FLAME Agent-Based Simulation Framework	EPSRC	Class1a	Prof Christopher Greenough	410	1	410
e207	Developing DL_POLY Molecular Dynamics Simulation code	EPSRC	Class1a	Dr Kostya Trachenko	25858	24294	1564
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26122	17022	9100
e226	Novel Vibrational Spectroscopic Techniques	EPSRC	Class1a	Dr Andrew D Burnett	1032	0	1032
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	20218	2054	18164
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50000	22152	27848

e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	1	499
e260	Microscopic gas diffusion-reaction model	EPSRC	Class1a	Dr Jochen Blumberger	4940	3385	1555
e266	Thermal and Reactive Flow Simulation on High-End Computers	EPSRC	Class1a	Prof Kai Luo	226800	9634	217166
e268	Modelling of marine renewable energy farms	EPSRC	Class1a	Dr Bjoern Elsaesser	10000	0	10000
e272	TOUCAN: Towards an Understanding of Catalysis on Nano-alloys	EPSRC	Class1a	Prof Roy L. Johnston	187000	12594	174406
e280	UK High-End Computing Consortium for Bio-molecular Simulation	EPSRC	Class1a	Prof. Adrian Mulholland	1075000	0	1075000
e281	Plasma Physics Consortium	EPSRC	Class1a	Dr Tony Arber	500000	3	499997
e282	SI2-CHE: Chemical Software	EPSRC	Class1a	Dr Lorna Smith	20472	8	20464
e283	UK Consortium on Mesoscopic Engineering Sciences	EPSRC	Class1a	Prof Kai Luo	403000	0	403000
e290	ExTASY	EPSRC	Class1a	Dr Charles Laughton	3524	0	3524
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71991	22904	48994
e235	Modelling offshore wind	EPSRC	Class1b	Prof Simon Watson	2100	1300	801
e249	Feedback flow control for reducing the aerodynamic drag	EPSRC	Class1b	Dr Aimee Morgans	9860	2961	6899
e254	Ceramic Composites for Fusion Power	EPSRC	Class1b	Prof Sergei Dudarev	8371	6582	1789

e258	Morphology and electronic props of semiconducting polymers	EPSRC	Class1b	Prof Alessandro Troisi	5650	5336	314
e270	Turbulent mass transfer at high Schmidt number	EPSRC	Class1b	Dr Maarten van Reeuwijk	17000	11115	5885
e271	Cloverleaf: preparing hydrodynamics codes for exascale	EPSRC	Class1b	Dr Stephen Jarvis	20430	18781	1649
e284	First Principles Modelling of Materials	EPSRC	Class1b	Dr Patrick R Briddon	20360	0	20360
e285	Modelling Fuel Droplets	EPSRC	Class1b	Prof Sergei Sazhin	890	5	886
e286	Investigation of wing stall delay effect	EPSRC	Class1b	Dr Alistair Revell	7068	0	7068
e287	Seeking Pathways to DFT studies of charge carriers	EPSRC	Class1b	Dr Christopher Castleton	1495	0	1495
e288	Image Similarity Metrics with Saliency Analysis	EPSRC	Class1b	Prof Richard Connor	1390	0	1390
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	4853	4810	43
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	22	378
e223	Numerical modelling of aorta dissection	EPSRC	Class2a	Prof. Xiaoyu Luo	300	0	300
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50	46	4
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400	399	1
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

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	221	179
e248	Testing of a Distributed Coordinate Descent Method	EPSRC	Class2a	Dr Peter Richtarik	400	112	288
e255	Turbulent Drag Reduction	EPSRC	Class2a	Dr Pierre Ricco	400	0	400
e256	Hybrid simulation on heat transfer	EPSRC	Class2a	Dr Huasheng Wang	300	39	261
e262	MC simulations of semiconductor nanostructures	EPSRC	Class2a	Prof Ian Galbraith	300	8	292
e264	Metabolic efficiency in neurons with extended morphology	EPSRC	Class2a	Dr Biswa Sengupta	300	214	86
e267	Simulating free-surface flow and fluid-structure interaction	EPSRC	Class2a	Dr Ido Akkerman	300	0	300
e274	Characterization of the dynamics of alpha-synuclein	EPSRC	Class2a	Prof Michele Vendruscolo	5739	440	5300
e275	Harmonic Generation in Time Dependent R-matrix Theory	EPSRC	Class2a	Dr Hugo van der Hart	300	148	152
e277	Cellular automata simulation of microstructure evolution	EPSRC	Class2a	Dr Anton Shterenlikht	300	17	283
e278	Ab-initio investigation of Beryllium intermetallic compounds	EPSRC	Class2a	Mr Patrick A Burr	300	276	24
e279	Characterisation of the triplet excited state potential	EPSRC	Class2a	Dr Paul Elliott	300	148	152

e289	Potential energy surface of the NO-N2 complex	EPSRC	Class2a	Dr Richard Wheatley	300	0	300
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1600	403	1197
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	325	476
e244	VOX-FE: Large Scale FE Bone Modelling on HECToR	EPSRC	Class2b	Prof Michael Fagan	800	8	792
e261	Expressive and scalable finite element simulation	EPSRC	Class2b	Dr Garth Wells	800	85	715
e265	HPC for the Discrete Element Method User Community	EPSRC	Class2b	Dr Catherine O'Sullivan	800	270	530
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	355962	244767	111195
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Grenville GMS Lister	884901	634138	250763
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	765655	582751	182904
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	254511	154927	99583
n99	NERC Training	NERC	Class1a	Dr Grenville GMS Lister	2	0	2
BBSRC Projects							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2000	1409	591
b100	Widening the BBSRC HPC User Base	BBSRC	Class1a	Dr Michael Ball	10000	641	9359
b12	Flu Analysis on HECToR	BBSRC	Class1a	Mr Adrian Jackson	50	0	50
b13	Linear Scaling DFT for Biochemistry Applications	BBSRC	Class1a	Dr David Bowler	5587	106	5482
b14	Understanding supercoiling-dependent DNA recognition	BBSRC	Class1a	Prof Anthony Maxwell	42600	31885	10715

b15	Simulating bird and dinosaur footprints	BBSRC	Class2a	Dr Peter L Falkingham	300	249	51
b16	First steps: velocity change in humans	BBSRC	Class1a	Dr Bill Sellers	18350	2720	15630
Director's Time							
b10	SPRINTing with HECToR [dCSE]	DT	Service	Mr Terry Sloan	4595	527	4068
d04	MSc in HPC	DT	Service	Dr David Henty	614	478	135
d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	10000	5848	4152
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	252	125	127
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1000	19	981
d24	SBSI	DirectorsTime	Service	Dr Stephen Gilmore	2000	958	1042
d25	Code Scaling	DirectorsTime	Service	Dr Ken Rice	51500	19033	32467
d26	Guest Training Accounts	DirectorsTime	Service	Miss Elizabeth Sim	1300	1225	75
d29	Nu-FuSe	DirectorsTime	Service	Mr Adrian Jackson	1500	939	561
d32	APOS-EU	DirectorsTime	Service	Dr Michele Weiland	1500	1000	501
d34	Msc 2011-2012	DirectorsTime	Service	Dr David Henty	1000	190	810
d35	PhD	DirectorsTime	Service	Dr Mark Bull	10	0	10
d36	Genome	DirectorsTime	Service	Dr Alan Gray	3460	0	3460
d37	CRESTA	DirectorsTime	Service	Dr Lorna Smith	21000	13188	7812

d39	NCSA access	DirectorsTime	Service	Mr Mark A Straka	1000	986	14
d40	Computational Chemistry at St Andrews	DirectorsTime	Service	Dr Herbert Fruchtl	2000	474	1526
d41	NPL Project	DirectorsTime	Service	Dr Ulrich Zachariae	90000	63116	26884
d42	Oxford Nanopore Technologies	DirectorsTime	Service	Dr Jayne Wallace	1170	734	436
d43	ECDF	DirectorsTime	Service	Mr Tony Weir	40000	20928	19072
d44	Crucible	DirectorsTime	Service	Mr Iain A Bethune	1000	0	1000
d45	MSc in HPC 2012-2013	DirectorsTime	Service	Dr David Henty	1000	267	733
d46	Silicate melts with CP2K	DirectorsTime	Service	Mr Iain A Bethune	500	0	500
d47	PGS Project	DirectorsTime	Service	Dr Kevin Stratford	100	0	100
d49	Leiden	DirectorsTime	Service	Dr. Simon Portegies Zwart	200	1	199
d50	Roslin Institute	DirectorsTime	Service	Mr Terry Sloan	400	0	400
d51	Superconducting Materials	DirectorsTime	Service	Dr Andreas Hermann	400	37	363
d52	Summer of HPC	DirectorsTime	Service	Mrs Irina Nazarova	500	0	500
External Projects							
e168	TEXT	External	Service	Dr Mark Bull	1500	80	1421

PRACE Projects							
pr1u0804	FULLDRUG	PRACE	DECI-8	Dr Chris A Johnson	15064	15063	1
pr1u0806	NELC	PRACE	DECI-8	Dr Chris A Johnson	11408	6709	4699
pr1u0807	PARAMETER	PRACE	DECI-8	Dr Chris A Johnson	14381	7074	7307
pr1u0809	VIPforVPH	PRACE	DECI-8	Dr Chris A Johnson	5346	1162	4184
pr1u0810	DrugEffluxMechanism	PRACE	DECI-8	Dr Chris A Johnson	4965	0	4965
pr1u0902	ESM4OED	PRACE	DECI-9	Dr Chris A Johnson	10272	6342	3930
pr1u0903	ICREIMUTANTS	PRACE	DECI-9	Dr Chris A Johnson	3766	792	2974
pr1u0904	MoMoGal	PRACE	DECI-9	Dr Chris A Johnson	7008	6515	493
pr1u0905	MPI-FETI	PRACE	DECI-9	Dr Chris A Johnson	9096	420	8676
pr1u0906	FORSQUALL	PRACE	DECI-9	Dr Chris A Johnson	3156	1	3155
pr1u1004	HIGHERFLY	PRACE	DECI-10	Dr Chris A Johnson	17120	365	16755
pr1u1008	HIV1-GSL	PRACE	DECI-10	Dr Chris A Johnson	23968	2679	21289
pr1u1009	INPHARMA	PRACE	DECI-10	Dr Chris A Johnson	2568	95	2473
pr1u1010	DNSTF	PRACE	DECI-10	Dr Chris A Johnson	28890	0	28890
pr1u1011	SPAITAC	PRACE	DECI-10	Dr Chris A Johnson	19067	5	19062
pr1u1012	NANODROPS	PRACE	DECI-10	Dr Chris A Johnson	27200	0	27200