HECToR Quarterly Report

Oct 2012 – Jan 2013

1 Introduction

This report covers the period from 1 October 2012 at 0800 to 1 January 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/4Q12.php

2 Executive Summary

- XE6 utilisation in 4Q12 was 69% compared to 67% in 3Q12. This equates to 87% of the optimum 80%. The Materials Chemistry Consortia (e05) used almost 25% of the AUs in the period. Further details are available in Section 3.2 of the report.

- There were 2 service failures in 4Q12. There was one blade voltage fault and one blower failure. The overall MTBF was the same as 3Q12 at 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 180TB (2.4%) is now in use.

- The 6 month trial of 24 hour queues continued in 4Q12. These jobs accounted for 18% of the utilisation in the quarter.

- A HECToR User meeting was held in December. Travel disruption resulted in some problems with speaker attendance however the meeting was well received.

3 Quantitative Metrics

3.1 Reliability

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

	Oct	Nov	Dec
Incidents	31	9	14
Failures	0	1	1

3.1.1 Performance Statistics

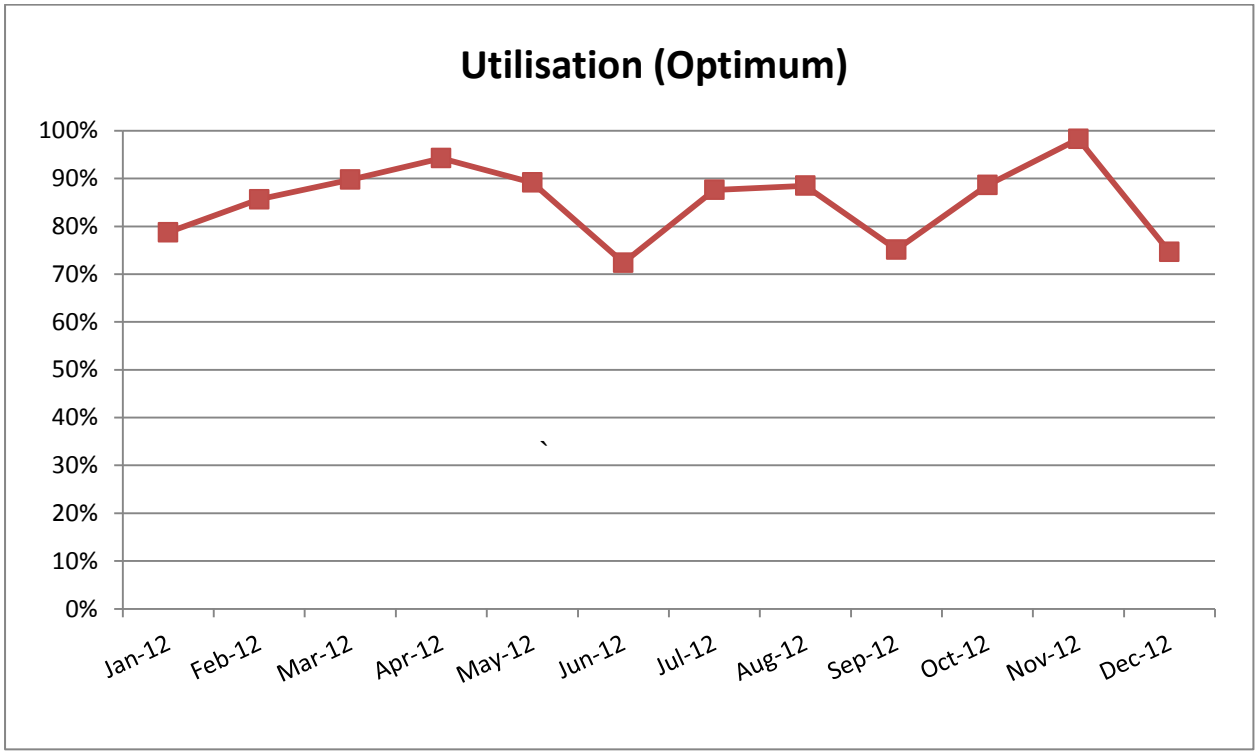
MTBF = (732)/(number of failures in a month)

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

Attribution	Metric	Oct	Nov	Dec	Quarterly
Technology	Failures	0	1	1	2
	MTBF	∞	732	732	1098
Service Provision	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	0	1	1	2
	MTBF	∞	732	732	1098

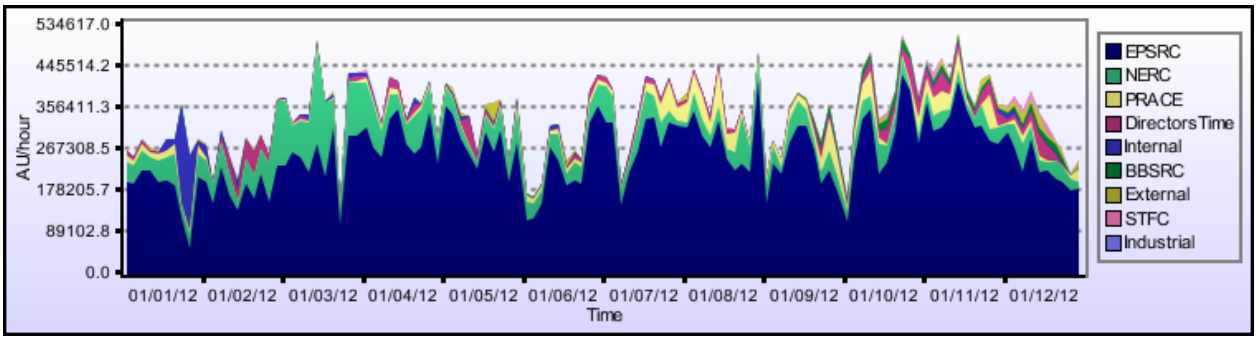
3.2 HECToR Utilisation

3.2.1 XE6 Utilisation



The XE6 utilisation quarterly average in 4Q12 was 87% of optimum, compared to 84% in 3Q12.

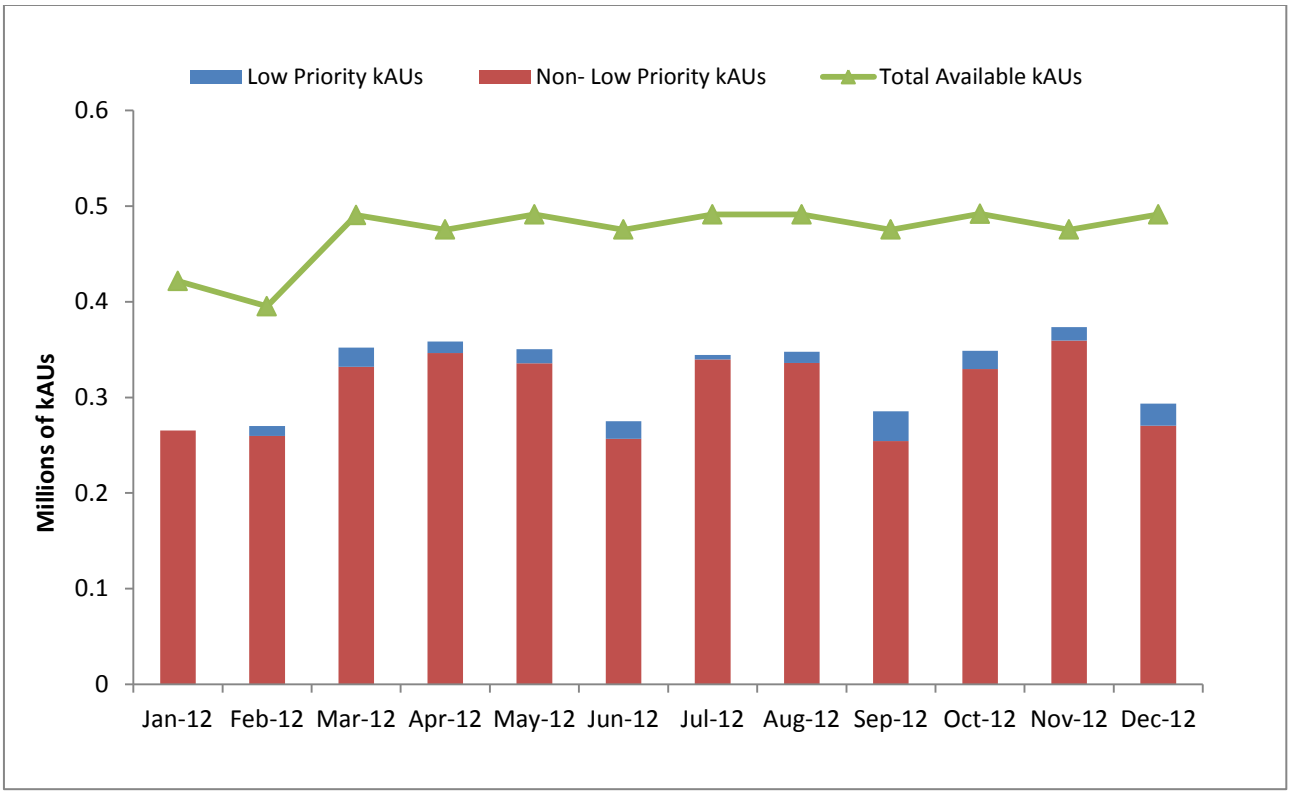
Capability Usage



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

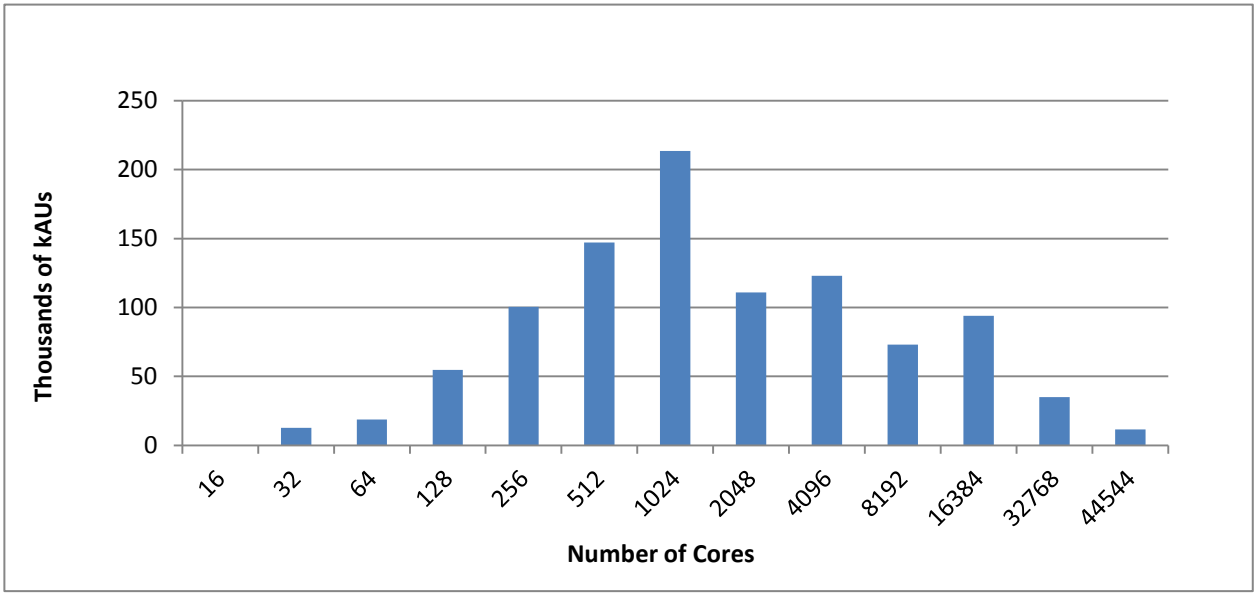
Low Priority Access

In 4Q12, low priority access accounted for 5.8% the overall utilisation.

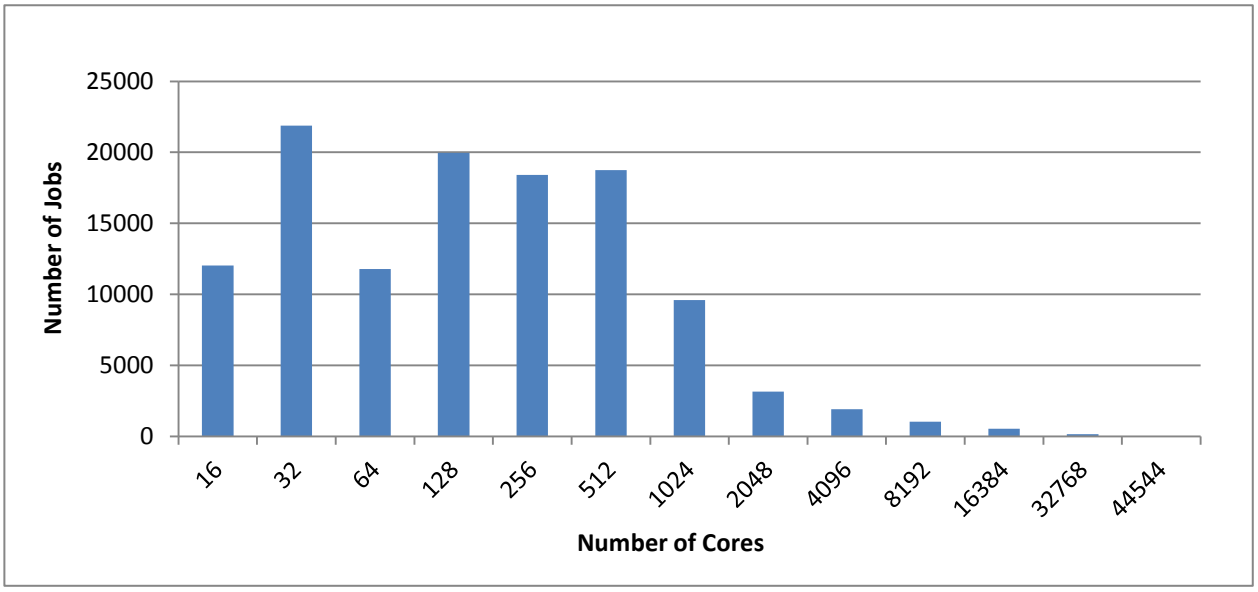


The low priority queue configuration will be reviewed with a view to increasing its effectiveness.

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
y02	20	49	170	0.0%
y03	576	682	655	0.1%
y04	0	0	2	0.0%
y07	2	3	52	0.0%
z01	105	181	285	0.0%
z03	2162	4053	770	0.3%
z06	2	4	16	0.0%
Internal Total	**2867**	**4972**	**1950**	**0.3%**
c01	2976	6918	1288	0.5%
e01	23756	68475	2803	4.7%
e05	192664	354330	28883	24.3%
e10	3104	5601	1636	0.4%
e19	0	0	1	0.0%
e71	4068	6963	314	0.5%
e82	2573	4404	89	0.3%
e89	13921	39438	3812	2.7%
e104	2907	5141	504	0.4%
e107	1055	2520	485	0.2%
e108	14572	25794	504	1.8%
e110	13178	23784	684	1.6%
e122	8251	14269	1556	1.0%
e124	0	0	2	0.0%
e125	1259	2156	112	0.2%
e126	207	355	2	0.0%
e127	1219	2087	90	0.1%
e128	0	0	1	0.0%
e129	331	566	26	0.0%
e130	7333	12554	281	0.9%
e141	285	580	262	0.0%
e145	25	43	20	0.0%
e149	710	1215	30	0.1%
e155	129	220	62	0.0%
e156	45	77	65	0.0%
e158	210	633	65	0.0%
e160	1592	2725	243	0.2%
e163	2050	3510	739	0.2%
e171	0	0	1	0.0%
e174	431	737	22	0.1%
e175	2096	15240	371	1.0%
e179	360	616	77	0.0%
e183	7323	12537	478	0.9%
e184	58	100	86	0.0%
e185	56	96	31	0.0%
e186	9949	18129	1509	1.2%
e187	22	38	121	0.0%
e192	3181	5445	230	0.4%
e202	14448	24734	492	1.7%
e203	2457	4207	274	0.3%

e204	1221	2090	74	0.1%
e206	1	1	51	0.0%
e207	239	511	3	0.0%
e213	1	2	2	0.0%
e228	347	595	89	0.0%
e229	1674	2865	5304	0.2%
e230	117	200	33	0.0%
e231	8	13	39	0.0%
e235	55	94	106	0.0%
e240	48	82	122	0.0%
e245	534	973	61	0.1%
e249	776	1329	122	0.1%
e251	2546	4383	54	0.3%
e252	12	21	28	0.0%
e253	11129	20040	113	1.4%
e254	60	205	2	0.0%
e257	1160	1987	116	0.1%
e258	3184	5450	94	0.4%
e259	9634	20401	120	1.4%
e260	932	1596	1085	0.1%
e261	0	1	23	0.0%
e262	0	1	33	0.0%
e263	2004	3431	170	0.2%
e264	118	202	12	0.0%
e267	0	0	28	0.0%
j01	0	0	5	0.0%
EPSRC Total	**374595**	**732704**	**56140**	**50.2%**
n01	13669	23400	4166	1.6%
n02	34862	60413	28134	4.1%
n03	19867	34014	7740	2.3%
n04	7010	12074	3511	0.8%
NERC Total	**75408**	**129900**	**43551**	**8.9%**
b14	14613	25016	1285	1.7%
b100	1	2	5	0.0%
BBSRC Total	**14613**	**25017**	**1290**	**1.7%**
p01	5486	9392	285	0.6%
STFC Total	**5486**	**9392**	**285**	**0.6%**
x01	9498	17032	5368	1.2%
External Total	**9498**	**17032**	**5368**	**1.2%**
b10	0	0	1	0.0%
d11	960	1794	559	0.1%
d15	9	15	116	0.0%
d25	4908	8403	945	0.6%
d26	59	68	338	0.0%
d27	58	100	142	0.0%
d29	524	1182	429	0.1%
d32	671	1241	510	0.1%
d37	3530	9956	657	0.7%
d39	0	1	24	0.0%
d40	26	44	43	0.0%
d41	15092	25836	3767	1.8%
d43	1141	1954	286	0.1%
d45	30	37	1239	0.0%
d47	0	0	3	0.0%

i04	44	75	7	0.0%
Directors Time Total	**27053**	**50705**	**9066**	**3.5%**
pr1u0702	1356	2321	102	0.2%
pr1u0704	2185	4759	288	0.3%
pr1u0705	210	360	43	0.0%
pr1u0706	9197	15745	256	1.1%
pr1u0804	2770	4742	196	0.3%
pr1u0805	6240	10683	260	0.7%
pr1u0806	371	635	103	0.0%
pr1u0807	75	129	84	0.0%
pr1u0808	2402	5195	9	0.4%
pr1u0809	34	59	2	0.0%
pr1u0902	532	911	130	0.1%
pr1u0903	12	21	9	0.0%
pr1u0904	134	229	44	0.0%
pr1u0905	51	87	74	0.0%
pr1u0906	1	2	12	0.0%
PRACE Total	**25571**	**45875**	**1612**	**3.2%**
i03	3	6	31	0.0%
x11	1	1	1	0.0%
Industrial Total	**4**	**7**	**32**	**0.0%**
Total	**535094**	**1015605**	**119294**	**69.6%**

3.3 Helpdesk

A total of 1251 queries with a specified service metric, and 118 queries with no metric were completed in this period.

Helpdesk Targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	1056	1064	99.2%	97.0%
Admin queries finished in 1 day	994	1001	99.3%	97.0%
Queries assigned in 30 min	1241	1251	99.2%	97.0%
Technical assessments in 10 days	46	46	100.0%	97.0%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	742	59.31%
Admin	259	20.70%
In-depth	141	11.27%
Technical	63	5.04%
Technical Assessment	46	3.68%

Queries by Category

Query Category	Queries	Percentage
New User	189	15.1%
New Password	129	10.3%
Set user quotas	112	9.0%
Set group quotas	99	7.9%
Access to HECToR	83	6.6%
None	69	5.5%
Disk, tapes, resources	61	4.9%
3rd Party Software	55	4.4%
Join Project	47	3.8%
Compilers and system software	46	3.7%
Add to group	42	3.4%
User behaviour	39	3.1%
New Group	39	3.1%
Batch system and queues	33	2.6%
Delete from project	30	2.4%
Other	27	2.2%
Login, passwords and ssh	26	2.1%
User programs	22	1.8%
Create certificate	21	1.7%
SAFE	16	1.3%
Update account	14	1.1%
Make Reservation	14	1.1%
Performance and scaling	8	0.6%
Node Failure	7	0.6%
Grid	5	0.4%
Delete Certificate	5	0.4%
Courses	5	0.4%
Network	4	0.3%
Static website	2	0.2%
Remove account	1	0.1%
Archive	1	0.1%

Queries by Handler Category

Handlers	Admin	Technical	Technical Assessment	Automatic	In-depth	Total	%age
CSE	1		46		65	112	8.95%
USL	230	42			54	326	26.06%
OSG	27	12		742	2	783	62.59%
Cray	1	9			20	30	2.40%

3.3.1 Quality Tokens

Seventeen positive quality tokens were received in 4Q12. There were no negative tokens.

Project	Positive Tokens	Comments
e05/x01	* * * *	
e01/e270	* * * *	*Pleased with service - look forward to performing further simulations*
e155	* * * *	*You fixed the certificate problem on hector/safe!*
x01	* * * * *	*Excellent service. I love HECToR.*

3.4 Performance Metrics

Metric	TSL(%)	FSL(%)	Oct-12	Nov-12	Dec-12	4Q12
Technology Reliability (%)	85.00%	98.50%	100.0%	99.6%	99.6%	99.7%
Technology MTBF (hours)	100	126.4	∞	732.0	732.0	1098.0
Technology Throughput, hours/year	7000	8367	8392.8	8599.0	8693.0	8564.4
Capability jobs completion rate	70%	90%	100.0%	100.0%	100.0%	100.0%
Non in-depth queries resolved within 1 day (%)	85%	97%	98.8%	99.8%	98.4%	99.2%
Number of SP FTEs	7.3	8.0	8.5	8.7	7.3	8.2
SP Serviceability (%)	80.00%	99.00%	100.0%	100.0%	100.0%	100.0%

Colour coding:

Exceeds FSL	
Between TSL and FSL	
Below TSL	

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	54804	53099	1705
e01	UK Turbulence Consortium	EPSRC	Class1a	Dr Gary N Coleman	490370	167496	322874
e05	Materials Chemistry HPC Consortium	EPSRC	Class1a	Prof C Richard A Catlow	1139874	978490	161324
e10	GENIUS	EPSRC	Class1a	Prof Peter Coveney	257748	24212	233537
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1a	Prof. Angelos Michaelides	50000	49888	113
e71	Simulating the control of calcite crystallisation	EPSRC	Class1a	Prof John Harding	130404	59373	71019
e76	HELIUM Developments	EPSRC	Class1a	Prof Ken Taylor	42522	40898	1624
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class1b	Dr Peter Haynes	4853	4233	620
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	400100	371684	28416
e122	Multiscale Modelling of Magnetised Plasma Turbulence	EPSRC	Class1a	Dr Colin M Roach	150000	84886	65114
e124	Compressible Axisymmetric Flows	EPSRC	Class1a	Prof Richard D Sandberg	22888	23224	-344
e125	Full configuration interaction quantum monte carlo	EPSRC	Class1a	Dr Ali Alavi	168325	39006	129209
e126	Clean Coal Combustion: Burning Issues of Syngas Burning	EPSRC	Class1a	Prof Xi Jiang	25584	17521	8064

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e127	Alternative drag-reduction strategies	EPSRC	Class1a	Prof Michael Leschziner	7000	4154	2846
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
e130	Novel hybrid LES-RANS schemes [MAN]	EPSRC	Class1a	Prof Dominique Laurence	10500	10489	11
e141	A numerical study of turbulent manoeuvering-body wakes	EPSRC	Class1a	Dr Gary N Coleman	16350	7458	8892
e145	UK-SHEC Consortium	EPSRC	Class1a	Dr T.J. Mays	1192	496	693
e149	Fractal-generated turbulence and mixing: flow physics and	EPSRC	Class1a	Prof Christos Vassilicos	68083	52807	15276
e155	Modelling Cholesterol Deposits	EPSRC	Class1a	Dr David Quigley	10000	1309	8691
e156	Metal Conquest: efficient simulation of metals on petaflop	EPSRC	Class2b	Dr David Bowler	1600	332	1268
e158	Novel Asynchronous Algorithms	EPSRC	Class1a	Prof Nicholas J Higham	2500	651	1849
e159	Multi-layered Abstractions for PDEs	EPSRC	Class1a	Prof Paul Kelly	3816	36	3780
e160	Sustainable Software Generation Tools	EPSRC	Class1a	Prof Paul Kelly	20208	15801	4407
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	Class1b	Dr Prashant Valluri	11495	3977	7518
e175	Fine-Scale Turbulence	EPSRC	Class1a	Prof Richard D Sandberg	50000	6755	43090
e179	Non-conservative dynamics	EPSRC	Class1a	Dr Daniel Dundas	87000	3071	83929

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e182	Advanced Modelling of Two-Phase Reacting Flow	EPSRC	Class1a	Dr Edward S Richardson	8150	0	8150
e183	Analysis of Processes in Hydrocarbon Fuel Droplets	EPSRC	Class1a	Prof Sergei Sazhin	8640	7944	696
e184	UK-RAMP	EPSRC	Class1a	Prof Ken Taylor	130500	1401	129099
e185	Chemistry of ceramic materials	EPSRC	Class1a	Prof John Harding	340000	6231	333769
e186	Step Change in Combustion Simulation	EPSRC	Class1a	Prof Kai Luo	70000	62556	7444
e187	IAGP: Integrated Assessment of Geoengineering Proposals	EPSRC	Class1a	Prof Piers Fosters	6030	657	5373
e191	CFD Analysis of Flight Dynamics	EPSRC	Class1a	Prof Kenneth Badcock	40500	4413	36087
e192	Physical properties of carbon nanotubes	EPSRC	Class1b	Dr Michael R C Hunt	10963	7203	3760
e202	Quantum Monte Carlo simulations	EPSRC	Class1a	Prof Matthew Foulkes	38345	14648	23697
e203	BeatBox - Realistic Cardiac Simulations	EPSRC	Class1a	Prof Vadim Biktashev	4500	4202	298
e204	Rare Events via Parallel Forward Flux Sampling	EPSRC	Class1a	Dr Rosalind Allen	5000	1645	3355
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	18040	7817
e213	Condensation/Evaporation Heat Transfer in Micro/Nanochannels	EPSRC	Class2a	Dr Huasheng Wang	400	10	390
e220	Study of interacting turbulent flames 2	EPSRC	Class1a	Dr N Swaminathan	26122	17022	9100
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	1032	0	1032

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e227	OPL	EPSRC	Class2a	Dr Radhika R. S. Saksena	50	46	4
e228	Development of the potential of doped metal-oxide nanotubes	EPSRC	Class1a	Dr Gilberto Teobaldi	20218	701	19517
e229	DTC in Complex Systems Simulations	EPSRC	Class1a	Prof Jonathan W Essex	50000	10331	39669
e235	Modelling offshore wind	EPSRC	Class1b	Prof Simon Watson	2100	539	1561
e237	Simulating Coupled Protein Folding and Nucleic Acid Binding	EPSRC	Class2a	Dr Christopher Baker	400	399	1
e240	MicroMag	EPSRC	Class2b	Prof Wyn Williams	800	314	486
e241	Potential Energy Surfaces for Bio-molecular Simulations	EPSRC	Class1a	Dr Lorna Smith	500	1	499
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	792
e245	Parallelisation of a harmonic balance NS solver	EPSRC	Class2b	Dr Sergio Campobasso	800	813	-13
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	102	298
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	501	7870
e255	Turbulent Drag Reduction	EPSRC	Class2a	Dr Pierre Ricco	400	0	400

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
e256	Hybrid simulation on heat transfer	EPSRC	Class2a	Dr Huasheng Wang	300	38	262
e257	Global stability and sensitivity of fuel injectors	EPSRC	Class1b	Dr. Matthew P Juniper	1728	1321	407
e258	Morphology and electronic props of semiconducting polymers	EPSRC	Class1b	Prof Alessandro Troisi	5650	4281	1369
e259	DNS of multi-species fuel combustion	EPSRC	Class1b	Dr N Swaminathan	31505	13644	17861
e260	Microscopic gas diffusion-reaction model	EPSRC	Class1a	Dr Jochen Blumberger	4940	1918	3022
e261	Expressive and scalable finite element simulation	EPSRC	Class2b	Dr Garth Wells	800	1	799
e262	MC simulations of semiconductor nanostructures	EPSRC	Class2a	Prof Ian Galbraith	300	2	298
e263	Modelling the Elastic and Moisture Barrier Properties of Skin	EPSRC	Class1b	Dr Rebecca Notman	40100	4051	36049
e264	Metabolic efficiency in neurons with extended morphology	EPSRC	Class2a	Dr Biswa Sengupta	300	118	182
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	226800	0	226800
e267	Simulating free-surface flow and fluid-structure interaction	EPSRC	Class2a	Dr Ido Akkerman	300	0	300
e268	Modelling of marine renewable energy farms	EPSRC	Class1a	Dr Bjoern Elsaesser	10000	0	10000
e269	Atomic data for fusion diagnostics	EPSRC	Class1b	Dr Catherine C A E Ramsbottom	4870	0	4870
e270	Turbulent mass transfer at high Schmidt number	EPSRC	Class1b	Dr Maarten van Reeuwijk	17000	0	17000
e271	Cloverleaf: preparing hydrodynamics codes for exascale	EPSRC	Class1b	Dr Stephen Jarvis	20430	0	20430
e272	TOUCAN: TOwards an Understanding of CAtalysis on Nanoalloys	EPSRC	Class1a	Prof Roy L. Johnston	187000	0	187000

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
j01	JST	EPSRC	Class1a	Dr Andrew R Turner	71991	22248	49650
STFC Projects							
p01	Atomic Physics for APARC	STFC	Class1a	Dr Penny Scott	10003	7630	2373
NERC Projects							
n01	Global Ocean Modelling Consortium	NERC	Class1a	Dr Andrew C Coward	255691	192952	62739
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1a	Dr Grenville GMS Lister	716228	529374	186854
n03	Computational Mineral Physics Consortium	NERC	Class1a	Prof John P Brodholt	558861	464028	94833
n04	Shelf Seas Consortium	NERC	Class1a	Dr Roger Proctor	157006	115156	41849
n99	NERC Training	NERC	Class1a	Dr Grenville GMS Lister	2	0	2
BBSRC Projects							
b09	Circadian Clock	BBSRC	Class1a	Prof Andrew A Millar	2000	1394	606
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	19740	22860
b15	Simulating bird and dinosaur footprints	BBSRC	Class2a	Dr Peter L Falkingham	300	0	300
Director's Time							

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d11	NAIS	DirectorsTime	Service	Prof Mark Ainsworth	10000	5530	4471
d15	HPC-GAP	DirectorsTime	Service	Dr David Henty	102	15	87
d21	GADGET	DirectorsTime	Service	Dr Adrian Jenkins	1000	19	981
d23	TEXT FP7	DirectorsTime	Service	Dr Mark Bull	1500	36	1464
d24	SBSI	DirectorsTime	Service	Dr Stephen Gilmore	2000	958	1042
d25	Code Scaling	DirectorsTime	Service	Dr Ken Rice	51500	17668	33832
d26	Guest Training Accounts	DirectorsTime	Service	Miss Elizabeth Sim	650	613	37
d29	Nu-FuSe	DirectorsTime	Service	Mr Adrian Jackson	1500	578	922
d30	PARTRAC	DirectorsTime	Service	Dr Mark Sawyer	200	124	76
d32	APOS-EU	DirectorsTime	Service	Dr Michele Weiland	1500	952	548
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	8236	12764
d38	Windfarm Simulation	DirectorsTime	Service	Mr Adrian Jackson	471	410	61
d39	NCSA access	DirectorsTime	Service	Mr Mark A Straka	1000	986	14
d40	Computational Chemistry at St Andrews	DirectorsTime	Service	Dr Herbert Fruchtl	2000	217	1784
d41	NPL Project	DirectorsTime	Service	Dr Ulrich Zachariae	45000	38739	6261

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d42	Oxford Nanopore Technologies	DirectorsTime	Service	Dr Jayne Wallace	1170	734	436
d43	ECDF	DirectorsTime	Class2b	Mr Tony Weir	13000	1698	11302
d44	Crucible	DirectorsTime	Service	Mr Iain A Bethune	1000	0	1000
d45	MSc in HPC 2012-2013	DirectorsTime	Service	Dr David Henty	1000	46	954
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	0	200
External Projects							
e168	TEXT	External	Service	Dr Mark Bull	1500	80	1421
x01	HPC-Europa	External	Service	Dr Judy Hardy	44762	43446	1317
PRACE Projects							
pr1u0702	HYDROGEN-ILs	PRACE	Class1a	Dr Chris A Johnson	770333	1699	768634
pr1u0704	HIFLY	PRACE	Class1a	Dr Chris A Johnson	8450	8499	-48
pr1u0705	TanGrin	PRACE	Class1a	Dr Chris A Johnson	14084	14042	42
pr1u0706	SIVE-2	PRACE	Class1a	Dr Chris A Johnson	14000	14411	-411
pr1u0804	FULLDRUG	PRACE	Class1a	Dr Chris A Johnson	15014	15063	-49
pr1u0805	NanoTherm	PRACE	Class1a	Dr Chris A Johnson	9009	9061	-51

Code	Project Title	Funding Body	Class	Principal Investigator	kAUs allocated	kAUs used	kAUs left
pr1u0806	NELC	PRACE	Class1a	Dr Chris A Johnson	11408	555	10853
pr1u0807	PARAMETER	PRACE	Class1a	Dr Chris A Johnson	6720	277	6443
pr1u0808	PIPETURB	PRACE	Class1a	Dr Chris A Johnson	12600	13511	-911
pr1u0809	VIPforVPH	PRACE	Class1a	Dr Chris A Johnson	5346	1162	4184
pr1u0810	DrugEffluxMechanism	PRACE	Class1a	Dr Chris A Johnson	4965	0	4965
pr1u0902	ESM4OED	PRACE	Class1a	Dr Chris A Johnson	10272	949	9323
pr1u0903	ICREIMUTANTS	PRACE	Class1a	Dr Chris A Johnson	3766	13	3754
pr1u0904	MoMoGal	PRACE	Class1a	Dr Chris A Johnson	23976	140	23836
pr1u0905	MPI-FETI	PRACE	Class1a	Dr Chris A Johnson	9096	63	9033
pr1u0906	FORSQUALL	PRACE	Class1a	Dr Chris A Johnson	3156	1	3155
pr1u0907	GPCR4D	PRACE	Class1a	Dr Chris A Johnson	2260	0	2260