HECToR Quarterly Report

July – September 2008

1. Introduction

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

Section 3 summarises service availability and performance statistics for this quarter. Section 4 shows utilisation of the service for the last six months. Section 7 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/3Q08.php

2. Executive Summary

- XT utilisation has remained relatively constant in 3Q08. The quarterly average was down slightly from 80% in 2Q08 to 70% in 2Q08. The capability challenge projects have again contributed significantly to overall utilisation. These projects are now coming to a close.

- 3Q08 was initially disappointing with a high number of service failures in July. These issues have now been addressed via firmware and configuration changes. August and September were much improved. The overall MTBF improved on 2Q08 from 169 to 220 hours. Single node failures continue to be a problem. No particular trend has been identified to date.

- The X2 Vector went live in July 2008 as planned. Early access users are now using the system. There have been no major issues to date. Utilisation in 3Q08 ~20%.

- A fix for the longstanding Lustre 4Tb quota limitation was successfully deployed on HECToR on 1st October. Both user and group quotas exceeding 4Tb can now be set.

- Options for the HECToR Phase2 upgrade including a combination of quad core and Baker are currently under review.

- The helpdesk statistics were again excellent. The volume of queries remained constant from 2Q08.

3. Availability

Failures

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

	July	*August*	*September*
Incidents	42	40	37
Failures	7	2	1

Single node failures dominate the above incidents. All node failures are tracked and work is ongoing to identify any trends in the root cause. In the event of a node failure, the affected users are notified by the Helpdesk and a refund is issued for the AUs lost.

Performance Statistics

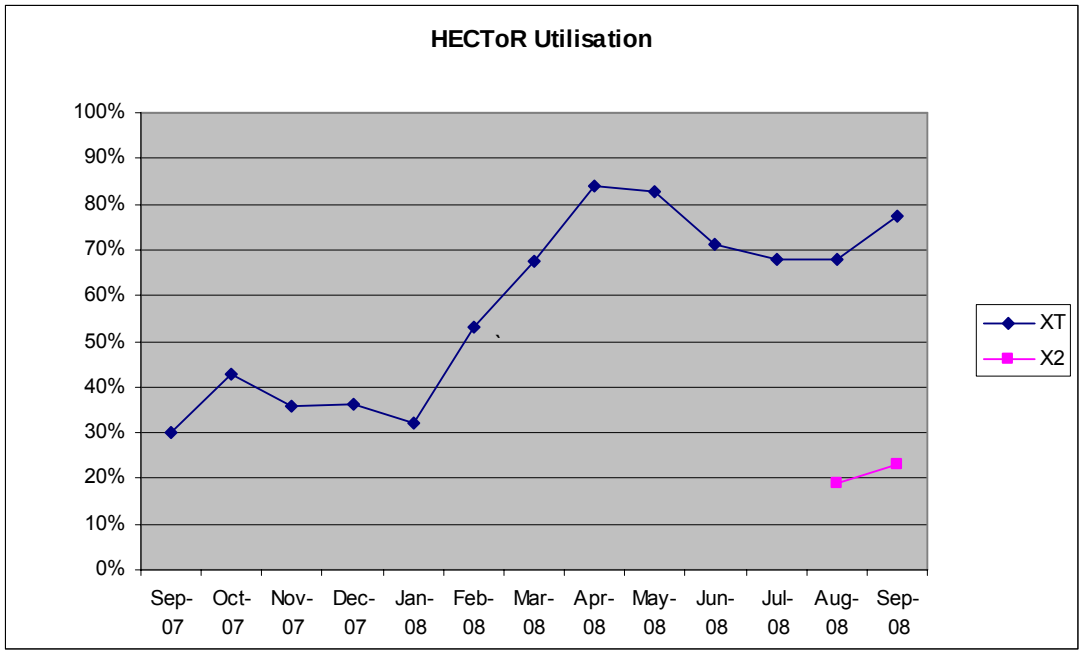
- MTBF = (732)/(number of failures in a month)

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

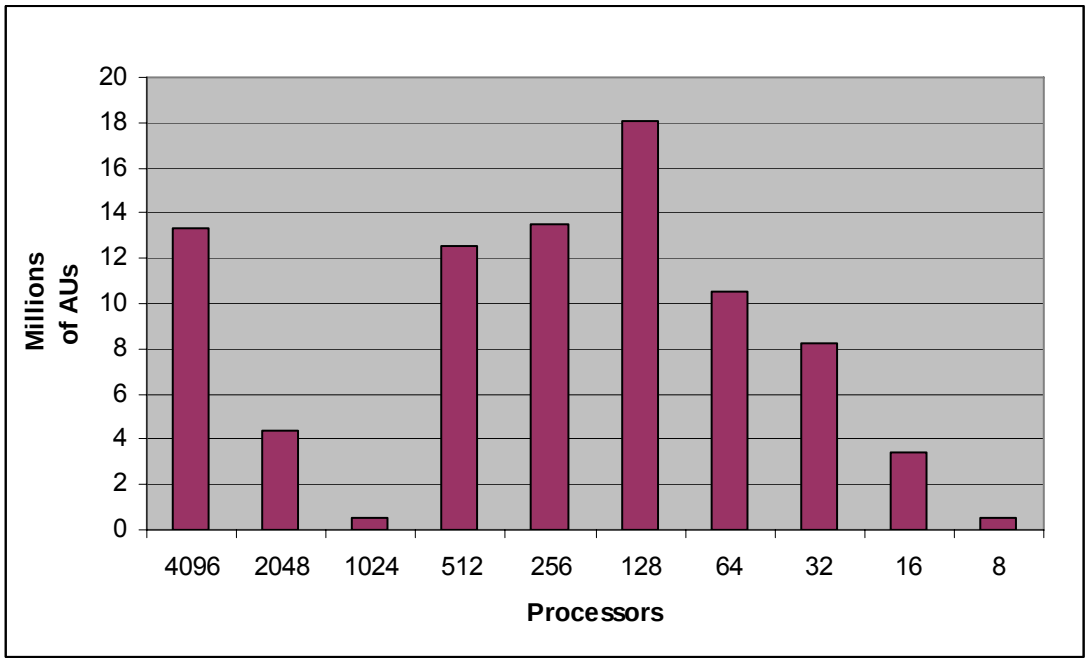
Attribution	*Metric*	*July*	*August*	*September*	*Quarterly*
Technology	Failures	7	1	0	8
	MTBF	105	732	∞	275
Service Provision	Failures	0	1	1	2
	MTBF	∞	732	732	1098
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	7	2	1	10
	MTBF	105	366	732	220

4. HECToR Utilisation

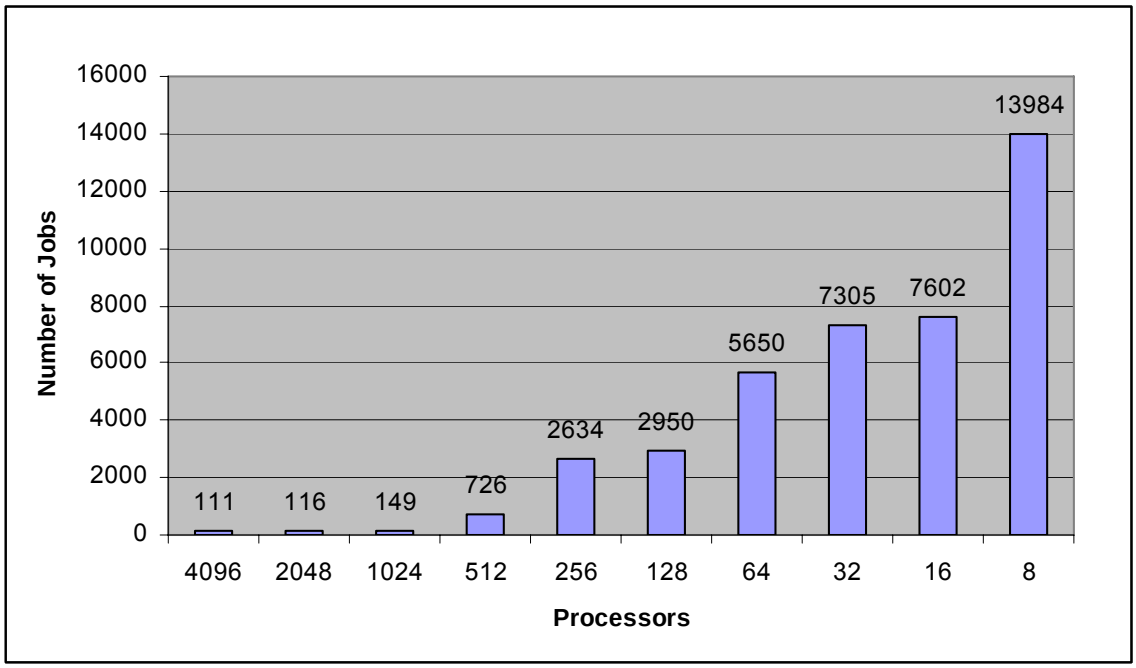
Overall Utilisation



XT Utilisation by queue



XT Number of jobs per queue



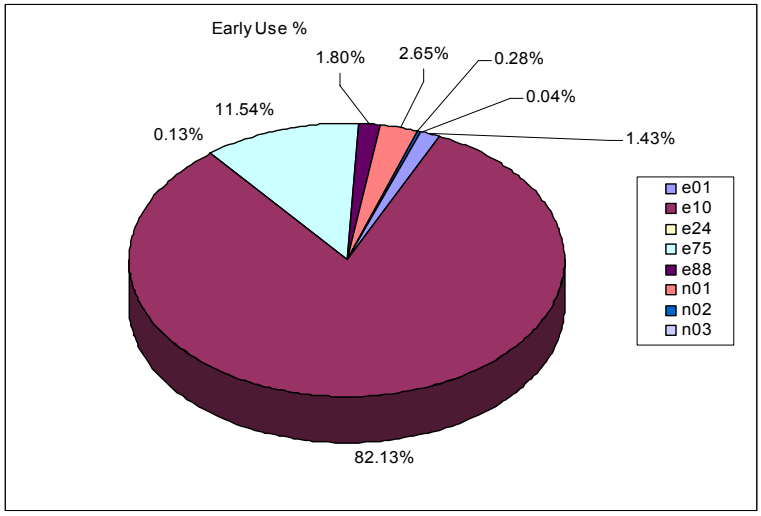
Usage by Consortium

Project	AUs	NJobs	%age of Use	Utilisation
c01	467,968	1316	0.5%	0.4%
e01	1,114,832	247	1.3%	0.9%
e05	2,391,477	2610	2.8%	2%
e10	195,208	432	0.2%	0.2%
e100	10	5	0%	0%
e24	686,143	1008	0.8%	0.6%
e34	465	9	0%	0%
e35	10,407	10	0%	0%
e42	239,094	284	0.3%	0.2%
e63	1,255,096	222	1.5%	1%
e68	3,845,157	3159	4.5%	3.2%
e69	8,221	246	0%	0%
e70	21,453	161	0%	0%
e71	7,478,175	1166	8.8%	6.2%
e72	4,814,134	3271	5.7%	4%
e73	6,902,397	712	8.1%	5.7%
e74	2,388,460	861	2.8%	2%
e75	6,832,521	384	8%	5.7%
e77	11,239	11	0%	0%
e78	37,021	21	0%	0%
e80	12,834,565	153	15.1%	10.6%
e82	23,676	141	0%	0%
e83	64,841	35	0.1%	0.1%
e87	2,312	8	0%	0%
e88	4,722,271	873	5.5%	3.9%
e89	9,091,113	2971	10.7%	7.5%
e90	17	54	0%	0%
e91	106,693	68	0.1%	0.1%
e92	23,298	98	0%	0%
e93	230,834	205	0.3%	0.2%
e94	4,779	24	0%	0%
e95	102,440	151	0.1%	0.1%
e98	9,386	39	0%	0%
e99	25,082	101	0%	0%
u02	16,546	287	0%	0%
u03	12,161	8	0%	0%
u10	348,595	268	0.4%	0.3%
EPSRC Total	**66,318,089**	**21619**	**77.90%**	**55%**
n01	1,498,978	1595	1.8%	1.20%
n02	6,305,709	7446	7.4%	5.20%
n03	10,565,431	2695	12.4%	8.80%
n04	109,937	219	0.1%	0.10%
u07	0	1	0%	0%
NERC Total	**18,480,056**	**11956**	**21.7%**	**15.30%**
x01	2,092	25	0%	0%
External Total	**2,092**	**25**	**0%**	**0%**
d01	5,179	15	0%	0%
d03	1,659	199	0%	0%
d04	18,413	676	0%	0%
Director's Time Total	**25,252**	**890**	**0%**	**0%**
Total	**85,148,164**	**42866**	**100%**	**70.6%**

5. X2 Utilisation

The X2 vector system went live in July 08 as planned. No major installation issues were encountered. Full accounting was enabled in August. X2 utilisation August/September was ~20%.

Early Access Usage



86% of early access use has been by EPSRC users. The table below shows the early access allocations and usage to date.

Code	Title	PI	X2 AUs allocated	X2 AUs used	X2 AUs left
EPSRC Projects					
e01	UK Turbulence Consortium	Dr Gary N Coleman	400,000	8,396	391,604
e10	GENIUS	Prof Peter Coveney	1,700,000	483,734	1,216,266
e75	Terascale DNS of Turbulence	Prof Christos Vassilicos	240,000	67,995	172,005
e88	Molecular Dynamics Simulation of a protein-ligand complex	Dr Charles Laughton	200,000	10,578	189,422
NERC Projects					
n01	Global Ocean Modelling Consortium	Dr Thomas Anderson	330,000	15,623	314,377
n02	NCAS (National Centre for Atmospheric Science)	Dr Lois Steenman-Clark	250,000	1,664	248,336
n03	Computational Mineral Physics Consortium	Prof John P Brodholt	250,000	228	249,772

6. Capability Challenge Projects

Although there has been small decrease since 2Q08, the 5 EPSRC Capability Challenge projects still accounted for 40% of the overall utilisation in 3Q08.

These projects have all now reached their end dates. Work is in progress with the PIs to ensure they have copies of the results before closing these out on HECToR.

The total AU usage of these projects is listed below.

Code	*PI*	*End Date*	*AUs Allocated*	*AUs Used*
e71	Harding	31/8/08	40,000,000	37,977,444
e72	Margetts	30/9/08	27,660,000	5,660,751
e73	Stratford	30/9/08	16,800,000	9,864,098
e74	Alfe	31/8/08	30,000,000	30,000,000
e80	Taylor	1/10/08	30,000,000	29,341,176

7. Helpdesk

A total of 892 queries with a specified service metric were completed in this period.

Helpdesk targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	736	741	99%	97%
Admin queries finished in 1 day	640	644	99%	97%
Queries assigned in 30 min	888	892	100%	97%
Technical assessments in 10 days	19	19	100%	97%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	456	51.1%
Admin	188	21.1%
In-depth	132	14.8%
Technical	97	10.9%
Technical assessment class-1	13	1.5%
Technical assessment class-2	6	0.7%

Queries by Category

Query Category	Queries	Percentage
New User	127	14.2%
Set user quotas	103	11.5%
Set group quotas	97	10.9%
Disk, tapes, resources	86	9.6%
3rd Party Software	63	7.1%
Compilers and system software	49	5.5%
Add to group	48	5.4%
New Password	47	5.3%
Access to HECToR	46	5.0%
None	45	5.0%
Batch system and queues	35	4.0%
Other	27	3.0%
User programs	26	2.9%
New Group	25	2.8%
User behaviour	17	1.9%
SAFE	13	1.5%
Login, passwords and ssh	12	1.3%
Join Project	8	0.9%

Performance and scaling	7	0.8%
Static website	3	0.3%
Grid	3	0.3%
Courses	3	0.3%
Porting	1	0.1%

Queries by Handler category

Handlers	Total	In-depth	Automatic	Technical	Admin	Technical assessment class-2	Technical assessment class-1	Percentage
CSE	64	53			1		10	7.2%
OSG	529	12	456	43	18			59.3%
USL	225	32		37	147	6	3	25.2%
Cray Systems	34	28		6				3.8%
Other	40	7		11	22			4.5%

8. Summary of Performance Metrics

Metric	TSL(%)	FSL(%)	Jul-08	Aug-08	Sep-08	3Q08
Technology reliability (%)	85.0%	98.5%	96.2	99.8	100.0	98.6
Technology MTBF (hours)	100.0	126.4	104.6	732.0	∞	220.0
Technology Throughput, hours/year	7000	8367	8311	8356	8476	8381
Capability jobs completion rate	70%	90%	91.3	100	100.0	96.3
Non in-depth queries resolved within 1 day (%)	85%	97%	100	98	100	99%
Number of SP FTEs	7.25	8.0	8.0	8.2	8.9	8.4
SP serviceability (%)	80.0%	99.0%	100.0	97.8	98.1	98.6

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							
c01	Support of EPSRC/STFC SLA	Class1	support	Dr Richard Blake	12,803,723	6,197,590	6,606,133
e01	UK Turbulence Consortium	Class1	Engineering	Dr Gary N Coleman	3,107,500	1,202,597	1,904,903
e05	Materials Chemistry HPC Consortium	Class1	Chemistry	Prof C Richard A Catlow	1,129,267,228	2,622,108	1,126,645,120
e10	GENIUS	Class1	Chemistry	Prof Peter Coveney	6,200,000	830,148	5,369,852
e100	Large scale MD and quantum embedding for biological systems	Class2	Materials	Prof Zheng X Guo	100,000	10	99,990
e101	Optimization of HPCx LES code	Class2	Engineering	Prof Michael Leschziner	100,000	0	100,000
e102	Numerical investigation of aerofoil noise	Class1	Engineering	Dr Richard D Sandberg	5,000,000	0	5,000,000
e103	Micromagnetic simulations on HPC architectures	Class2	Engineering	Dr Hans Fangohr	100,000	0	100,000
e104	Fluid-Mechanical Models applied to Heart Failure	Class1	Physics	Dr Nicolas Smiths	2,400,000	0	2,400,000
e24	DEISA	Class1	support	Mrs Alison Kennedy	20,702,294	1,498,486	19,203,808
e34	Hydrogen vacancy distribution in magnesium hydride	Class2	Chemistry	Prof Nora de Leeuw	100,000	465	99,535
e35	Non-adiabatic processes	Class1	Materials	Dr Tchavdar Todorov	1,000,000	15,718	984,282
e42	Computational Combustion for Engineering Applications	Class1	Engineering	Prof Kai Luo	32,000,000	2,437,130	29,562,870
e63	UK Applied Aerodynamics Consortium 2	Class1	Engineering	Dr Nick Hills	13,500,000	2,315,058	11,184,942
e68	Hydrogenation Reactions at Metal Surfaces	Class1	Chemistry	Dr Angelos Michaelides	50,000,000	12,734,222	37,265,778
e69	Simulations of a Subsonic Cylindrical Cavity Flow	Class2	Engineering	Dr Aldo Rona	100,000	31,312	68,688
e70	Computation of Electron Transfer Properties	Class1	Chemistry	Dr Jochen Blumberger	960,000	33,953	926,047
e71	Simulating the control of calcite crystallisation	Class1	Chemistry	Prof John Harding	40,000,000	38,208,779	1,791,221
e72	Ultrascalable Modelling of Materials	Class1	Materials	Dr Lee Margetts	27,660,000	6,514,783	21,145,217

e73	Tera-scale Shear Flow Challenge	Class1	Materials	Dr Kevin Stratford	16,800,000	10,797,542	6,002,458
e74	Quantum Monte Carlo Methods	Class1	Materials	Prof Dario Alfe`	30,000,000	31,530,229	-1,530,229
e75	Terascale DNS of Turbulence	Class1	Engineering	Prof Christos Vassilicos	27,760,000	20,634,273	7,125,727
e76	HELIUM Developments	Class1	Physics	Prof Ken Taylor	6,000,000	0	6,000,000
e77	Porting of DFT/GW Codes	Class2	Engineering	Prof M M DeSouza	60,000	40,993	19,007
e78	Q-Espresso CP/PWSCF Codes on HECToR	Class2	Chemistry	Dr Antonio Tilocca	100,000	91,091	8,909
e79	SMEAGOL	Class1	Physics	Prof Colin Lambert	3,000,000	20	2,999,980
e80	Double Ionisation of Helium	Class1	Physics	Prof Ken Taylor	30,000,000	30,347,190	-347,190
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	23,676	76,324
e83	Ab initio study of high pressure disordered ice	Class2	Physics	Dr Simon P Bates	100,000	100,589	-589
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	2,312	97,688
e88	Molecular Dynamics Simulation of a protein-ligand complex	Class1	Chemistry	Dr Charles Laughton	10,200,000	7,288,204	2,911,796
e89	Support for UK Car-Parrinello Consortium	Class1	Physics	Dr Matt Probert	140,000,000	10,166,692	129,833,308
e90	Network modelling of wireless cities	Class2	Engineering	Prof Jonathan M Pitts	100,000	17	99,983
e91	Bulk properties of TiO2-B as lithium battery anodes	Class2	Chemistry	Prof M Saiful Islam	100,000	106,693	-6,693
e92	Dynamo Action In Compressible Convection	Class2	Physics	Mr Paul Bushby	75,000	23,299	51,701
e93	ACE - Architecture Exercise	Service	support	Dr Lorna Smith	500,000	508,677	-8,677
e94	Porting the Linear Scaling DTF Code Conquest to HECToR	Class2	Physics	Dr David Bowler	100,000	5,473	94,527
e95	Novel Apatite Materials	Class2	Materials	Prof M Saiful Islam	100,000	102,440	-2,440
e96	Materials Property Relationships	Class2	Materials	Dr Shoufeng Yang	100,000	0	100,000
e97	Discovery of innovative hydrogen storage materials	Class2	Chemistry	Prof Zheng X Guo	100,000	0	100,000

e98	Non-linear magnetohydrodynamic modelling of tokamak plasmas	Class2	Physics	Mr Ian T Chapman	100,000	9,386	90,614
e99	New Developments in Modelling Electron Energy Loss Spectroscopy	Class2	Materials	Mr Andrew J Scott	100,000	35,647	64,353
u02	Materials simulation using AIMPRO	Early use	Materials	Dr Patrick R Briddon	4,000,000	3,077,672	922,328
u03	DNS of NACA-0012 aerofoil at Mach 0.4	Early use	Engineering	Dr Gary N Coleman	2,500,000	2,299,119	200,881
u06	Modelling of Protein Flexibility Upon Ligand Binding	Early use	Chemistry	Prof Jonathan W Essex	1,900,000	1,906,861	-6,861
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	2,013,446	486,554
u11	Ice Nucleation and Growth	Early use	Environment	Prof Mark Rodger	1,000,000	993,256	6,744
y08	Testing	Early use	support	Dr David Jenkins	1,000	0	1,000
NERC Projects							
n01	Global Ocean Modelling Consortium	Class1	Environment	Dr Thomas Anderson	9,830,000	4,241,741	5,588,259
n02	NCAS (National Centre for Atmospheric Science)	Class1	Environment	Dr Lois Steenman-Clark	52,000,000	16,772,919	35,227,081
n03	Computational Mineral Physics Consortium	Class1	Environment	Prof John P Brodholt	72,779,000	43,081,321	29,697,679
n04	Shelf Seas Consortium	Class1	Environment	Dr Roger Proctor	8,250,000	180,832	8,069,168
u01	Melting of MgSiO3 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
STFC Projects							
u08	UKQCD	Early use	Physics	Dr Jonathan Flynn	8,000,000	7,969,011	30,989
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							
T01	NIMES: New Improved Muds from Environmental Sources.	Class1	Environment	Dr Chris Greenwell	4,113,669	0	4,113,669
x01	HPC-Europa	Class1	External	Dr Judy Hardy	375,000	113,213	261,787
Director's Time							
d01	UKQCD-DT	Early use	Physics	Dr Jonathan Flynn	4,007,024	3,968,926	38,098
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	11,940	988,060
d04	MSc Projects	Service	External	Dr David Henty	93,000	26,465	66,535
d05	Icon-DT	Service	Engineering	Mr Paul Graham	250,000	0	250,000
d06	LSST-DT	Service	Engineering	Mr Davy Virdee	10,000	0	10,000
y09	Director's Time	Service	External	Prof Arthur S Trew	82,538	82,538	0