HECToR Quarterly Report

October - December 2008

1. Introduction

This report covers the period from 1 October 2008 at 0800 to 1 January 2009 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 6 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/4Q08.php

2. Executive Summary

- XT utilisation has decreased during 4Q08. The quarterly average was down from 70% in 3Q08 to 57% in 4Q08. The end of the capability challenge projects in 3Q08 has contributed to this decrease. The festive holiday period also impacts overall 4Q08 statistics. A number of BBSRC projects which were previously using HPCx have recently transitioned across to HECToR. The results from the current dCSE call are due in late January which should also lead to some new projects on HECToR.

- Reliability was disappointing in 4Q08. Out of the 11 service failures, 6 of them were Lustre related. Patches have since been provided by Cray and were applied to the filesystem in early January. The overall MTBF decreased slightly on 3Q08 from 220 to 200 hours.

- Single node failures continue to be a problem. 3 recurring faults are being further investigated by Cray but as yet no root cause has been identified.

- The X2 Vector system was very reliable in 4Q08. Utilisation remained fairly constant from the previous quarter at 22%. All users were contacted with regard to transferring machine time from the XT to the X2 but as yet there has been no take up on this.

- Proposals for the HECToR Phase 2 upgrade have been submitted to EPSRC and H-SAC and we are currently waiting formal approval from EPSRC.

- The helpdesk statistics were again excellent. The volume of queries remained constant from 3Q08.

3. Availability

Failures

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

	October	*November*	*December*
Incidents	23	25	35
Failures	3	3	5

Lustre filesystem errors accounted for 6 of the 11 Failures. Patches have since been provided and applied to the system in early January.

Single node failures dominate the above incidents. There are three main areas being investigated by Cray but as yet no root cause or fix has been identified.

Performance Statistics

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

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

Attribution	*Metric*	*October*	*November*	*December*	*Quarterly*
Technology	Failures	3	3	4	10
	MTBF	244	244	183	220
Service Provision	Failures	0	0	1	1
	MTBF	∞	∞	732	2196
External	Failures	0	0	0	0
	MTBF	∞	∞	∞	∞
Overall	Failures	3	3	5	11
	MTBF	244	244	146	200

4. HECToR Utilisation

Overall Utilisation
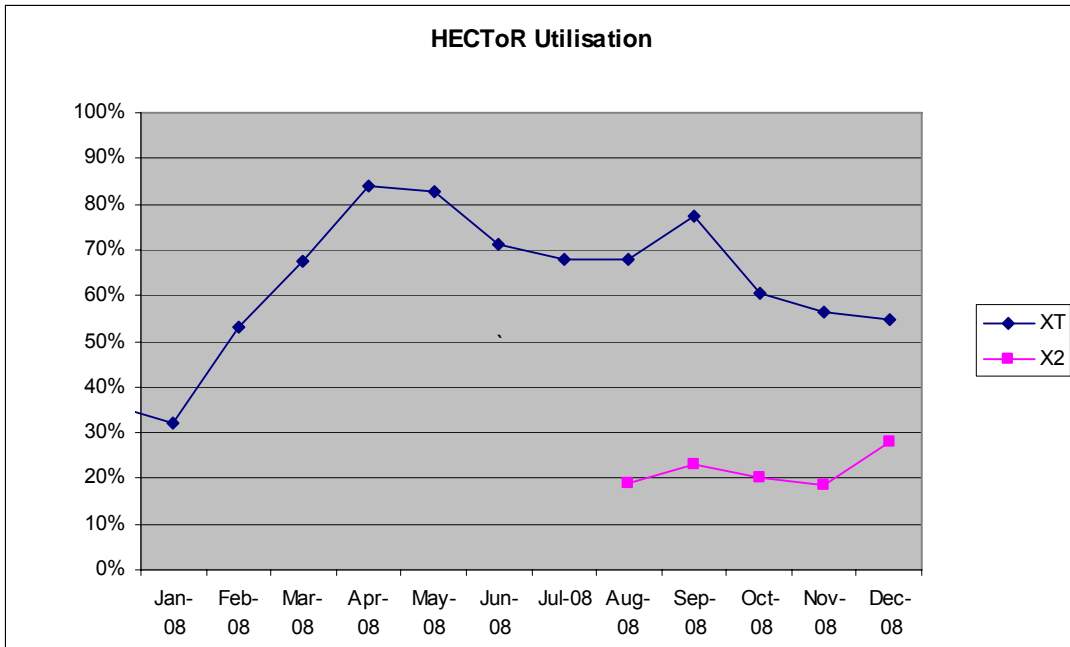
XT Utilisation by queue
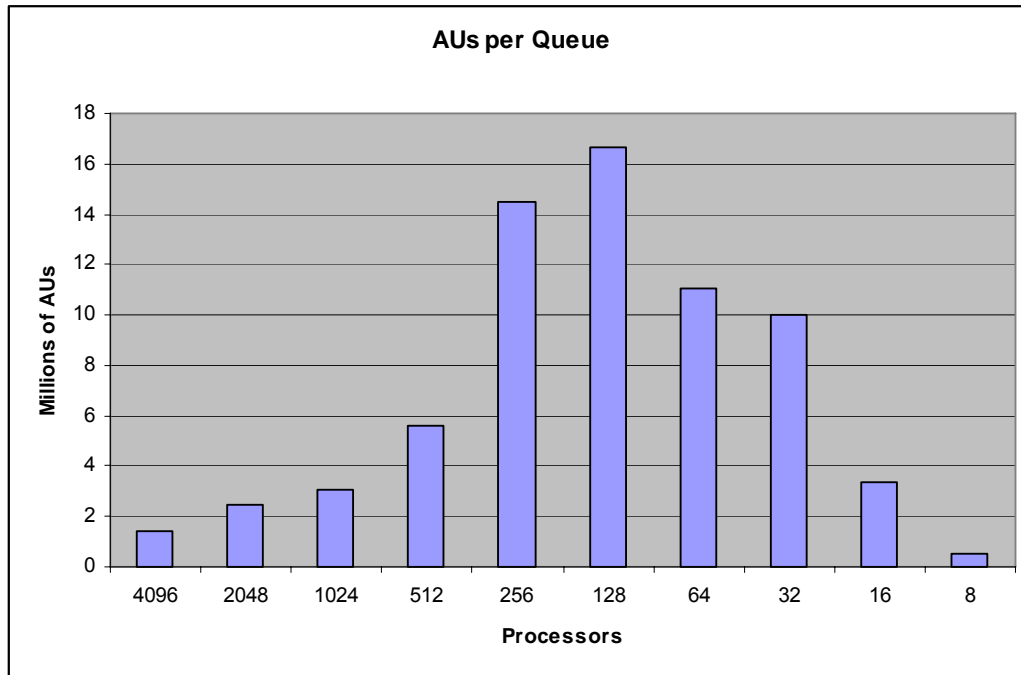
AUs per Queue

XT Number of jobs per queue

Number of jobs per queue
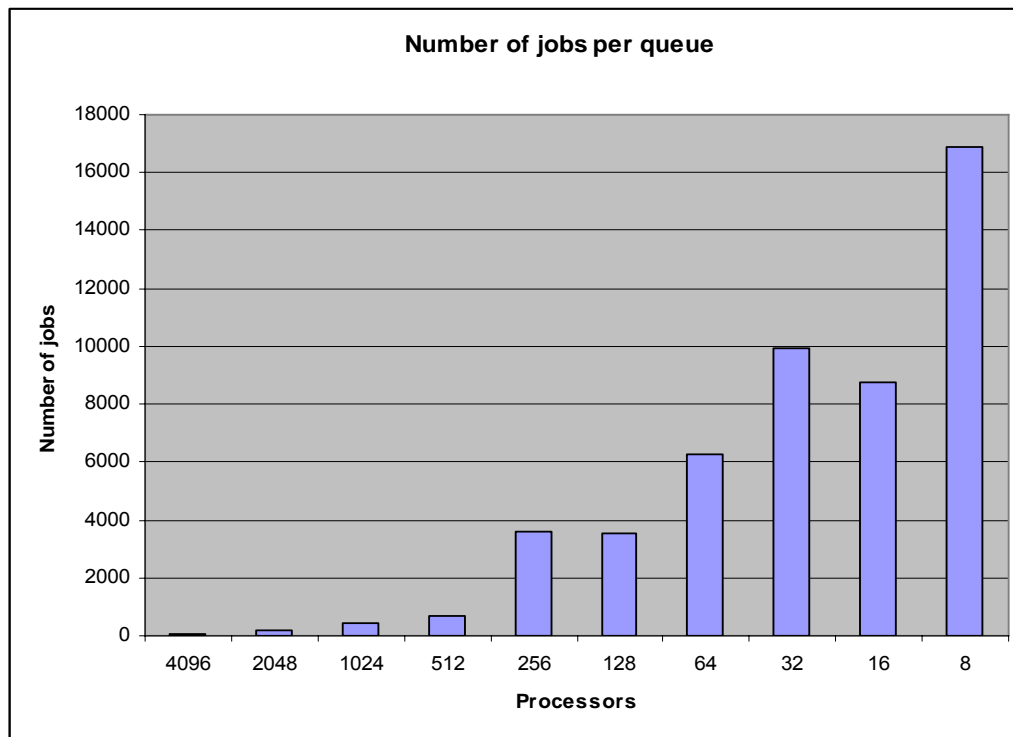
Usage by Consortium

Project	AUs	NJobs	%age of Use	Utilisation
y01	0	3	0%	0%
y02	583,268	2726	0.8%	0.5%
y03	0	1010	0%	0%
y04	14	26	0%	0%
y05	3,808	109	0%	0%
y06	13	2356	0%	0%
y07	0	19	0%	0%
z01	165,860	1230	0.2%	0.1%
z02	25	6	0%	0%
z03	109,014	2553	0.2%	0.1%
Internal Total	862,002	10038	1.2%	0.7%
c01	423,899	813	0.6%	0.4%
e01	183,545	89	0.3%	0.2%
e05	3,492,852	3452	5.1%	2.9%
e10	4,215,097	1443	6.1%	3.5%
e102	15,165	30	0%	0%
e109	0	1	0%	0%
e24	6,969,081	3627	10.1%	5.8%
e34	14,437	76	0%	0%
e35	18,096	50	0%	0%
e42	1,361,155	1227	2%	1.1%
e59	16,321	222	0%	0%
e63	1,319,536	570	1.9%	1.1%
e68	6,895,179	3173	10.0%	5.7%
e69	40,132	265	0.1%	0%
e70	111,213	227	0.2%	0.1%
e71	1,889,813	221	2.7%	1.6%
e72	1,961,231	2073	2.8%	1.6%
e73	430,685	90	0.6%	0.4%
e74	947,091	32	1.4%	0.8%
e75	4,737,148	206	6.9%	3.9%
e76	1,682,903	152	2.4%	1.4%
e78	1,628	12	0%	0%
e80	664,376	31	1.0%	0.6%
e81	100	249	0%	0%
e82	67,052	149	0.1%	0.1%
e87	89,051	43	0.1%	0.1%
e88	2,956,116	790	4.3%	2.4%
e89	7,285,567	2464	10.6%	6%
e90	270	29	0%	0%
e92	27,558	14	0%	0%
e93	3	1	0%	0%
e94	97	8	0%	0%
e98	15,733	54	0%	0%
e99	79,579	240	0.1%	0.1%
u02	2,771	175	0%	0%
u03	1,930	92	0%	0%
u10	121,778	289	0.2%	0.1%
u11	64	1	0%	0%
EPSRC Total	48,038,250	22680	69.6%	39.8%
n01	1,549,931	1643	2.2%	1.3%

n02	9,756,206	13407	14.1%	8.1%
n03	7,286,697	3080	10.6%	6%
n04	879,360	933	1.3%	0.7%
NERC Total	19,472,194	19063	28.2%	16.1%
b01	1	11	0%	0%
BBSRC Total	1	11	0%	0%
T01	6,178	115	0%	0%
x01	370,132	503	0.5%	0.3%
External Total	376,311	618	0.5%	0.3%
d03	1,961	104	0%	0%
d05	30,583	26	0%	0%
d07	263,587	46	0.4%	0.2%
DirectorsTime Total	296,131	176	0.4%	0.2%
Total	**69,044,889**	**52586**	**100%**	**57.20%**

X2 Utilisation

Project	AUs	NJobs	%age of Use	Utilisation
y02	2,153	85	0.20%	0%
y03	0	21	0%	0%
z01	147,703	291	14%	3.10%
z03	37,131	630	3.50%	0.80%
z06	233	123	0%	0%
Internal Total	187,220	1150	17.70%	3.90%
e01	364,218	475	34.40%	7.70%
e10	345,359	51	32.60%	7.30%
e24	1,098	79	0.10%	0%
e75	144,847	402	13.70%	3%
EPSRC Total	855,521	1007	80.90%	18%
n01	443	24	0%	0%
n02	12,736	305	1.20%	0.30%
n03	1,143	37	0.10%	0%
NERC Total	14,321	366	1.40%	0.30%
d04	979	6	0.10%	0%
DirectorsTime Total	979	6	0.10%	0%
Total	**1,058,042**	**2529**	**100%**	**22.30%**

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	373,988	26,011
e10	GENIUS	Prof Peter Coveney	1,700,000	841,318	858,681
e75	Terascale DNS of Turbulence	Prof Christos Vassilicos	240,000	229,913	10,086
e88	Molecular Dynamics Simulation of a protein-ligand complex	Dr Charles Laughton	200,000	10,578	189,421
n01	Global Ocean Modelling Consortium	Dr Thomas Anderson	330,000	16,065	313,934
n02	NCAS (National Centre for Atmospheric Science)	Dr Lois Steenman-Clark	750,000	15,651	734,348
n03	Computational Mineral Physics Consortium	Prof John P Brodholt	250,000	1,370.4732	248,629

6. Helpdesk

A total of 983 queries with a specified service metric were completed in this period.

Helpdesk targets

Metric	Pass	Total	Fraction	Target
All queries finished in 1 day	820	828	99%	97%
Admin queries finished in 1 day	734	742	99%	97%
Queries assigned in 30 min	983	983	100%	97%
Technical assessments in 10 days	30	30	100%	97%

Queries by Service Metric

Service Metric	Queries	Percentage
Automatic	475	48.3%
Admin	267	27.2%
In-depth	125	12.7%
Technical	86	8.7%
Technical assessment class-1	24	2.4%
Technical assessment class-2	6	0.6%

Queries by Category

Query Category	Queries	Percentage
New User	134	13.60%
Set user quotas	114	11.60%
User behaviour	97	9.90%
Set group quotas	70	7.10%
Add to group	70	7.10%
Disk, tapes, resources	62	6.30%
New Password	49	5%
Access to HECToR	49	5%
None	44	4.50%
Node Failure	38	3.90%
3rd Party Software	38	3.90%
Batch system and queues	37	3.80%
Compilers and system software	32	3.30%
User programs	31	3.20%
Login, passwords and ssh	17	1.70%
SAFE	16	1.60%
Other	16	1.60%

New Group	16	1.60%
Join Project	12	1.20%
Courses	10	1%
Performance and scaling	9	0.90%
Delete from group	6	0.60%
Static website	5	0.50%
Network	3	0.30%
Grid	3	0.30%
Porting	2	0.20%
Create certificate	2	0.20%
Remove account	1	0.10%

Queries by Handler category

Handlers	Total	Admin	Automatic	Technical	In-depth	Technical assessment class-1	Technical assessment class-2	Percentage
Other	81	49		22	7	2	1	8.2%
USL	272	199	1	29	38	2	3	27.7%
OSG	526	15	474	28	9			53.5%
Cray Systems	18	1		7	10			1.8%
CSE	86	3			61	20	2	8.7%

8. Summary of Performance Metrics

Metric	TSL(%)	FSL(%)	Oct-08	Nov-08	Dec-08	4Q08
Technology reliability (%)	85.00%	98.50%	97.80%	99.20%	98.50%	98.50%
Technology MTBF (hours)	100	126.4	244	244	183	200
Technology Throughput, hours/year	7000	8367	8378	8575	8257	8403
Capability jobs completion rate	70%	90%	98.40%	92.00%	100.00%	97.70%
Non in-depth queries resolved within 1 day (%)	85%	97%	99%	100%	98%	99%
Number of SP FTEs	7.3	8.0	8.7	8.0	8.0	8.2
SP Serviceability (%)	80.00%	99.00%	100.00%	100.00%	99.40%	99.80%

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

EPSRC Projects								
c01	Support of EPSRC/STFC SLA	EPSRC	Class1	support	Dr Richard Blake	12,803,723	6,753,052	6,050,671
e01	UK Turbulence Consortium	EPSRC	Class1	Engineering	Dr Gary N Coleman	3,107,500	1,672,366	1,435,134
e05	Materials Chemistry HPC Consortium	EPSRC	Class1	Chemistry	Prof C Richard A Catlow	1,129,267,228	6,419,663	1,122,847,565
e10	GENIUS	EPSRC	Class1	Chemistry	Prof Peter Coveney	9,257,856	5,436,742	3,821,114
e100	Large scale MD and quantum embedding for biological systems	EPSRC	Class2	Materials	Prof Zheng X Guo	100,000	10	99,990
e101	Optimization of HPCx LES code	EPSRC	Class2	Engineering	Prof Michael Leschziner	100,000	0	100,000
e102	Numerical investigation of aerofoil noise	EPSRC	Class1	Engineering	Dr Richard D Sandberg	5,000,000	69,097	4,930,903
e103	Micromagnetic simulations on HPC architectures	EPSRC	Class2	Engineering	Dr Hans Fangohr	100,000	0	100,000
e104	Fluid-Mechanical Models applied to Heart Failure	EPSRC	Class1	Physics	Dr Nicolas Smiths	2,400,000	0	2,400,000
e105	Joint Euler/Lagrange Method for Multi-Scale Problems	EPSRC	Class1	Engineering	Dr Andreas M Kempf	1,300,000	0	1,300,000
e106	Numerical Simulation of Multiphase Flow: From Mesocales to	EPSRC	Class1	Engineering	Prof Kai Luo	3,650,000	0	3,650,000
e107	Parallel Brain Surgery Simulation	EPSRC	Class1	Life Sciences	Dr Stephane P. A. Bordas	6,000,000	1	5,999,999
e108	Unsteady Propeller Noise	EPSRC	Class2	Engineering	Dr Sergey Karabasov	100,000	0	100,000
e109	Nonlinear modelling of tokamak plasma eruptions	EPSRC	Class2	Physics	Prof Howard Wilson	100,000	0	100,000
e110	Computational Aeroacoustics Consortium	EPSRC	Class1	Engineering	Prof Paul Tucker	39,000,000	0	39,000,000
e111	The Modelling of New Catalysts for Fuel Cell Application	EPSRC	Class2	Physics	Prof Dario Alfe`	100,000	0	100,000

e24	DEISA	EPSRC	Class1	support	Mrs Alison Kennedy	21,902,294	8,336,942	13,565,352
e34	Hydrogen vacancy distribution in magnesium hydride	EPSRC	Class2	Chemistry	Prof Nora de Leeuw	100,000	14,902	85,098
e35	Non-adiabatic processes	EPSRC	Class1	Materials	Dr Tchavdar Todorov	3,000,000	29,939	2,970,061
e42	Computational Combustion for Engineering Applications	EPSRC	Class1	Engineering	Prof Kai Luo	32,000,000	4,137,540	27,862,460
e59	Turbulence in Breaking Gravity Waves	EPSRC	Class1	Engineering	Prof Ian P Castro	400,000	18,319	381,681
e63	UK Applied Aerodynamics Consortium 2	EPSRC	Class1	Engineering	Dr Nick Hills	13,500,000	3,647,748	9,852,252
e68	Hydrogenation Reactions at Metal Surfaces	EPSRC	Class1	Chemistry	Dr Angelos Michaelides	50,000,000	20,163,250	29,836,750
e69	Simulations of a Subsonic Cylindrical Cavity Flow	EPSRC	Class2	Engineering	Dr Aldo Rona	100,000	81,812	18,188
e70	Computation of Electron Transfer Properties	EPSRC	Class1	Chemistry	Dr Jochen Blumberger	960,000	132,753	827,247
e72	Ultrascalable Modelling of Materials	EPSRC	Class2	Materials	Dr Lee Margetts	8,622,547	8,459,577	162,970
e74	Quantum Monte Carlo Methods	EPSRC	Class1	Materials	Prof Dario Alfe`	30,008,735	32,477,320	-2,468,585
e75	Terascale DNS of Turbulence	EPSRC	Class1	Engineering	Prof Christos Vassilicos	27,760,000	24,890,344	2,869,656
e76	HELIUM Developments	EPSRC	Class1	Physics	Prof Ken Taylor	6,000,000	1,861,801	4,138,199
e78	Q-Espresso CP/PWSCF Codes on HECToR	EPSRC	Class2	Chemistry	Dr Antonio Tilocca	100,000	91,184	8,816
e79	SMEAGOL	EPSRC	Class1	Physics	Prof Colin Lambert	3,000,000	20	2,999,980
e81	e-Collision experiments using HPC	EPSRC	Class2	Physics	Prof NS Scott	200,000	100	199,900
e82	ONETEP: linear-scaling method on High Performance Computers	EPSRC	Class2	Materials	Dr Peter Haynes	100,000	90,727	9,273
e83	Ab initio study of high pressure disordered ice	EPSRC	Class2	Physics	Dr Simon P Bates	100,000	100,589	-589
e84	Vortical Mode Interactions	EPSRC	Class1	Engineering	Dr Tamer Zaki	3,200,000	16	3,199,984
e85	Study of Interacting Turbulent Flames	EPSRC	Class1	Engineering	Dr N Swaminathan	2,083,000	0	2,083,000

e86	Single molecule vibrational microscopy and spectroscopy	EPSRC	Class2	Materials	Prof Andrew Fisher	100,000	103,105	-3,105
e87	Model Parameters for Unsaturated Elasto-plastic Models	EPSRC	Class2	Engineering	Dr Charles Augarde	100,000	91,363	8,637
e89	Support for UK Car-Parrinello Consortium	EPSRC	Class1	Physics	Dr Matt Probert	140,000,000	17,936,482	122,063,518
e90	Network modelling of wireless cities	EPSRC	Class2	Engineering	Prof Jonathan M Pitts	100,000	286	99,714
e92	Dynamo Action In Compressible Convection	EPSRC	Class2	Physics	Mr Paul Bushby	75,000	50,856	24,144
e94	Porting the Linear Scaling DTF Code Conquest to HECToR	EPSRC	Class2	Physics	Dr David Bowler	100,000	5,570	94,430
e96	Materials Property Relationships	EPSRC	Class2	Materials	Dr Shoufeng Yang	100,000	0	100,000
e97	Discovery of innovative hydrogen storage materials	EPSRC	Class2	Chemistry	Prof Zheng X Guo	100,000	0	100,000
e98	Non-linear magnetohydrodynamic modelling of tokamak plasmas	EPSRC	Class2	Physics	Mr Ian T Chapman	100,000	25,680	74,320
e99	New Developments in Modelling Electron Energy Loss Spectroscopy	EPSRC	Class2	Materials	Mr Andrew J Scott	100,000	138,818	-38,818
u02	Materials simulation using AIMPRO	EPSRC	Early use	Materials	Dr Patrick R Briddon	4,000,000	3,080,443	919,557
u03	DNS of NACA-0012 aerofoil at Mach 0.4	EPSRC	Early use	Engineering	Dr Gary N Coleman	2,500,000	2,301,049	198,951
u10	Turbulent Plasma Transport in Tokamaks	EPSRC	Early use	Physics	Dr Colin M Roach	2,500,000	2,121,848	378,152
y08	Testing	EPSRC	Early use	support	Dr David Jenkins	1,000	0	1,000
NERC projects								
n01	Global Ocean Modelling Consortium	NERC	Class1	Environment	Dr Thomas Anderson	9,830,000	6,143,815	3,686,185
n02	NCAS (National Centre for Atmospheric Science)	NERC	Class1	Environment	Dr Lois Steenman-Clark	52,500,000	26,927,314	25,572,686
n03	Computational Mineral Physics Consortium	NERC	Class1	Environment	Prof John P Brodholt	72,779,000	50,739,382	22,039,618
n04	Shelf Seas Consortium	NERC	Class1	Environment	Dr Roger Proctor	8,250,000	1,296,940	6,953,060

BBSRC projects								
b01	Biomarkers for patient classification	BBSRC	Class2	Life Sciences	Prof. Peter Ghazal	100,000	1	99,999
b08	Int BioSim	BBSRC	Class1	Life Sciences	Mr Mark M Sansom	866,000	0	866,000
b09	Circadian Clock	BBSRC	Class1	Materials	Prof Andrew A Millar	2,000,000	0	2,000,000
External projects								
x01	HPC-Europa	External	Class1	External	Dr Judy Hardy	375,000	483,338	-108,338
T01	NIMES: New Improved Muds from Environmental Sources.	External	Class1	Environment	Dr Chris Greenwell	4,113,669	19,910	4,093,759
Director's Time								
d03	EUFORIA	Directors Time	Service	Physics	Mr Adrian Jackson	1,000,000	24,559	975,441
d04	MSc Projects	Directors Time	Service	External	Dr David Henty	93,000	27,444	65,556
d05	Icon-DT	Directors Time	Service	Engineering	Mr Paul Graham	250,000	68,990	181,010
d07	Thermal ellipsiods and proton transfer	Directors Time	Service	Chemistry	Dr Carole A Morrison	1,116,000	265,788	850,212
d08	Oncology	Directors Time	Service	Chemistry	Mr Florian Scharinger	35,000	1,264	33,736
y09	Director's Time	Directors Time	Service	External	Prof Arthur S Trew	846,708	82,538	764,170