

HPCx Service Report

September 2006

1 Introduction

This report covers the period from 0800 on 30 September 2006 to 0800 on 1 October 2006, a service month of 720 hours.

Utilisation of the main service exceeded 80% for the second month in a row and reached 81.9%. More than a third of main service utilisation was by NERC projects.

2 Usage

2.1 Availability

Incidents

During this month, there were 5 incidents, one of which was at SEV1. The following table indicates the severity levels of the incidents, where SEV 1 is defined as a *Failure* (in contractual terms). The definitions used for severity levels can be found in Appendix A.

<i>Severity</i>	<i>Number</i>
1	1
2	2
3	2
4	0

The MTBF figures for this month were as follows:

<i>SEV1</i>	<i>Incidents</i>	<i>MTBF</i>
IBM	0.0	∞
Site	1.0	720
External	0.0	∞
<i>Overall</i>	1.0	720

The following table gives more details on the Severity 1 incidents:

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
06.089	100%	0%	0%	Emergency power off after aircon failure

Serviceability

Scheduled downtime for this month was 13.0 hours.

<i>Attribution</i>	<i>UDT</i>	<i>Serviceability</i>
IBM	0:00	100.0
Site	4:00	99.4
External	0:00	100.0
<i>Overall</i>	4:00	99.4

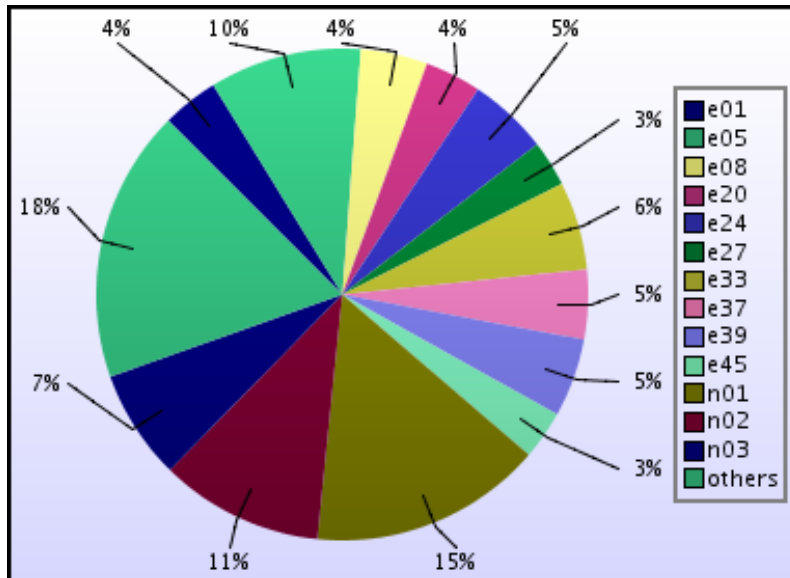
2.2 CPU Usage by Consortium

Main Service

<i>Consortium</i>	<i>CPU Hours (Parallel)</i>	<i>CPU Hours (Other)</i>	<i>AUs charged</i>	<i>%age of charged AUs</i>
e01	31552	222	152976	3.7%
e03	127	0	613	0.0%
e05	84495	981	410995	10.0%
e06	22961	348	112218	2.7%
e08	37649	0	181259	4.4%
e11	14036	0	67577	1.6%
e14	13388	112	64997	1.6%
e15	359	1	1731	0.0%
e17	3564	12	17219	0.4%
e20	31600	0	152136	3.7%
e23	349	0	1681	0.0%
e24	44852	0	215940	5.2%
e25	0	3	14	0.0%
e27	25759	0	124014	3.0%
e31	0	1	2	0.0%
e33	49595	0	238773	5.8%
e35	1969	52	9730	0.2%
e36	760	0	3661	0.1%
e37	39039	1	187956	4.6%
e38	196	0	946	0.0%
e39	44118	42	212602	5.2%
e42	4643	2	22361	0.5%
e45	27296	0	131413	3.2%
e49	8687	5	41848	1.0%
e50	3321	0	15987	0.4%
e51	26	0	125	0.0%
e52	0	0	1	0.0%
e53	320	46	1764	0.0%
e54	0	6	32	0.0%
e56	11182	0	53834	1.3%
<i>EPSRC Total</i>	<i>501844</i>	<i>1834</i>	<i>2424403</i>	<i>58.9%</i>
n01	130934	31	630522	15.3%

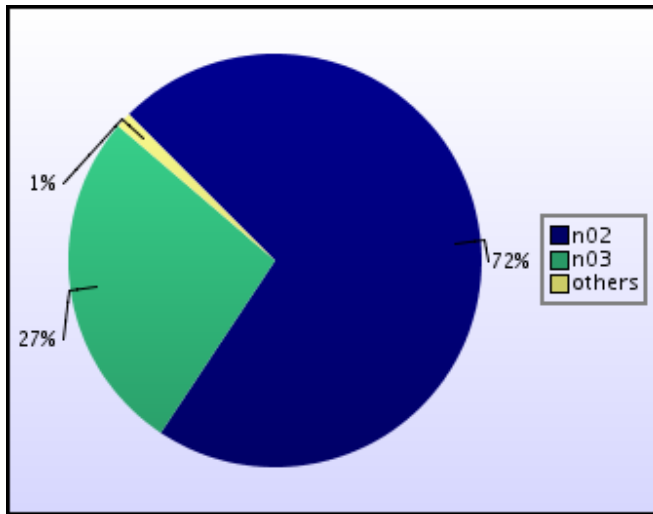
n02	91768	12	441871	10.7%
n03	61714	23	297226	7.2%
n04	8656	6	41699	1.0%
<i>NERC Total</i>	293071	71	1411318	34.3%
p01	17511	1	84310	2.0%
<i>PPARC Total</i>	17511	1	84310	2.0%
c01	15893	18	76600	1.9%
<i>CCLRC Total</i>	15893	18	76600	1.9%
b08	1142	335	7109	0.2%
<i>BBSRC Total</i>	1142	335	7109	0.2%
x01	1502	19	7320	0.2%
<i>External Total</i>	1502	19	7320	0.2%
z001	9362	19	45165	1.1%
z002	0	0	1	0.0%
z004	144	0	694	0.0%
z06	12106	0	58285	1.4%
<i>HPCx Total</i>	21612	19	104144	2.5%

Use by project



Development Service

<i>Consortium</i>	<i>CPU Hours (Parallel)</i>	<i>CPU Hours (Other)</i>	<i>AUs charged</i>	<i>%age of charged AUs</i>
n01	194	0	935	0.1%
n02	98443	317	475474	71.8%
n03	37079	0	178516	27.0%
n04	1466	17	7137	1.1%
<i>NERC Total</i>	137182	333	662062	100.0%



2.3 CPU Usage by Job Type

The figures for *Raw AUs* given here show the number of AUs actually supplied by the system to users' jobs.

Main service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	330041	8.0%	2516
33–64	281967	6.9%	561
65–128	729471	17.8%	381
129–256	1713573	41.7%	683
257–512	986492	24.0%	125
513–1024	5814	0.1%	27
>1024	57316	1.4%	20

Utilisation by region

The regions of the main service are:

- Capacity Region (26 nodes, for jobs using ≤128 CPUs)
- Capability Region (64 nodes, principally for jobs using >128 CPUs)
- Interactive-parallel Region (2 nodes)

At present, when there are many 128-processor jobs waiting to use the capacity region, the systems team responds by moving such jobs into the capability region, if there is room there. As a result, relative utilisation figures for the regions do not provide significantly useful information.

Overall utilisation of the main service was 81.9%.

Development Service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	468757	71.0%	3351
33–64	184056	27.9%	1307
65–128	7579	1.1%	27
129–256	67	0.0%	1

On 17 August 2006, 8 nodes were added to this region in order to exercise them as part of the preparation for Phase 3, increasing the number of processors from 192 to 320.

These nodes were still in operation in the period from 8 am on 1 September to 8 am on 12 September, making an extra 177480 AUs available this month. The overall utilisation of the enlarged development service was 79.5%, equivalent to 101.1% of the normally-available AUs. This continues the trend of increasing utilisation of this service.

2.4 Slowdown and Job Wait Times

Slowdowns

Slowdown is a widely used measure of the relative wait times of different classes of jobs. It is defined as:

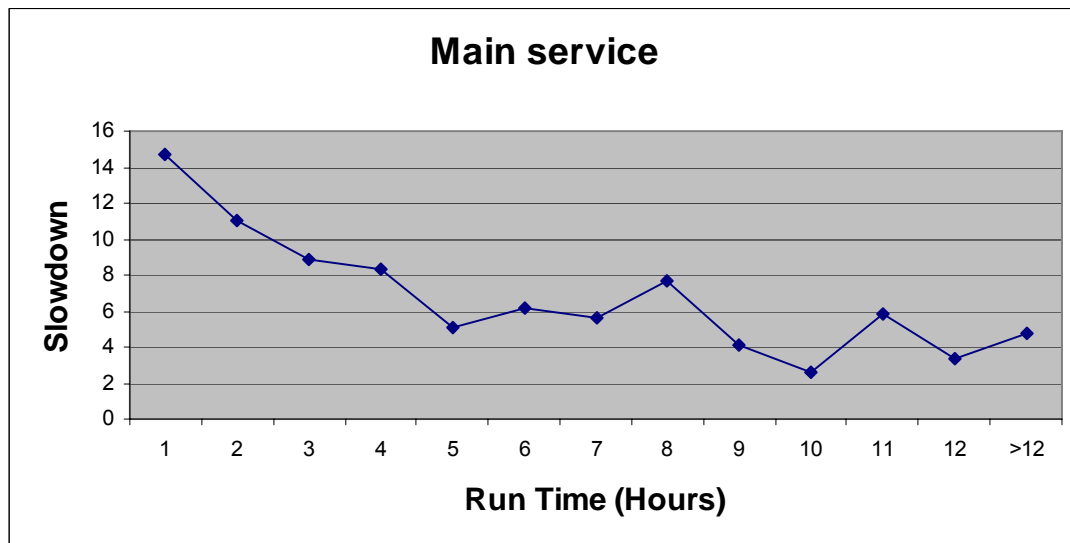
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

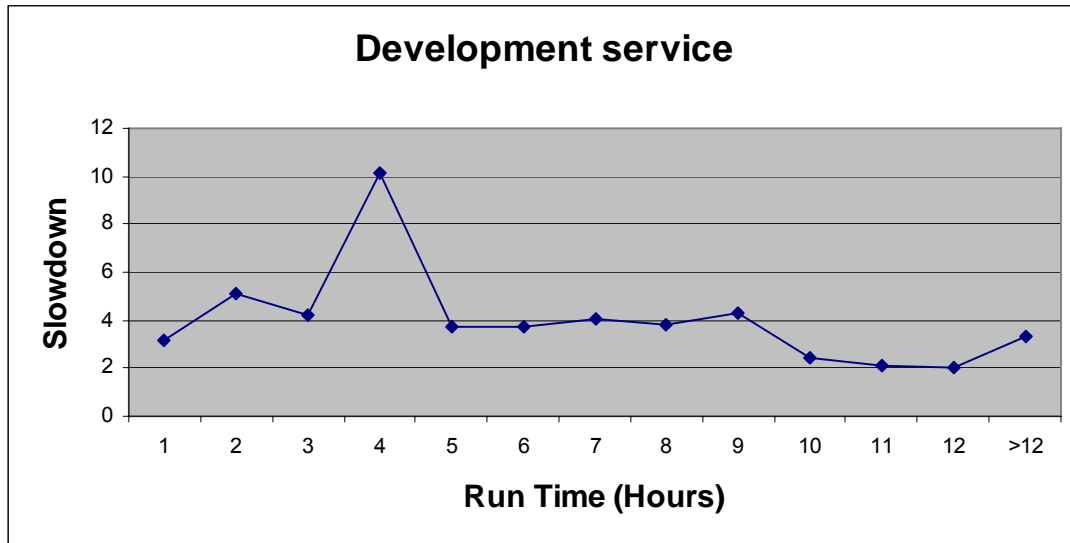
Slowdowns of less than around 10 are usually regarded as reasonable.

On both services, slowdowns are currently satisfactory.

Slowdowns by runtime

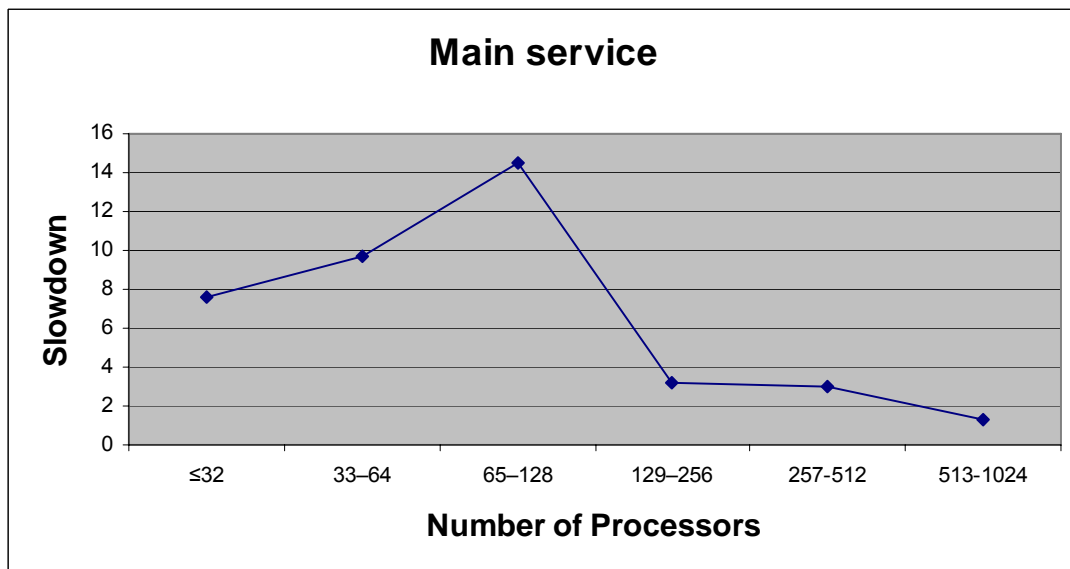
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

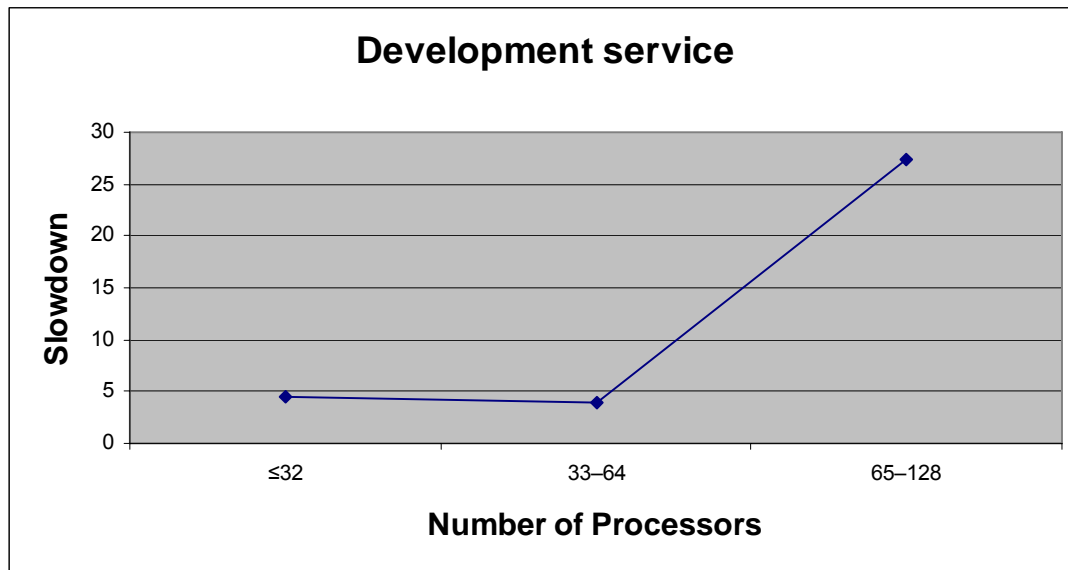




Slowdowns by number of processors

In the graphs below, we plot the slowdown figures against the number of processors used. Jobs which ran for less than 1 hour are ignored.



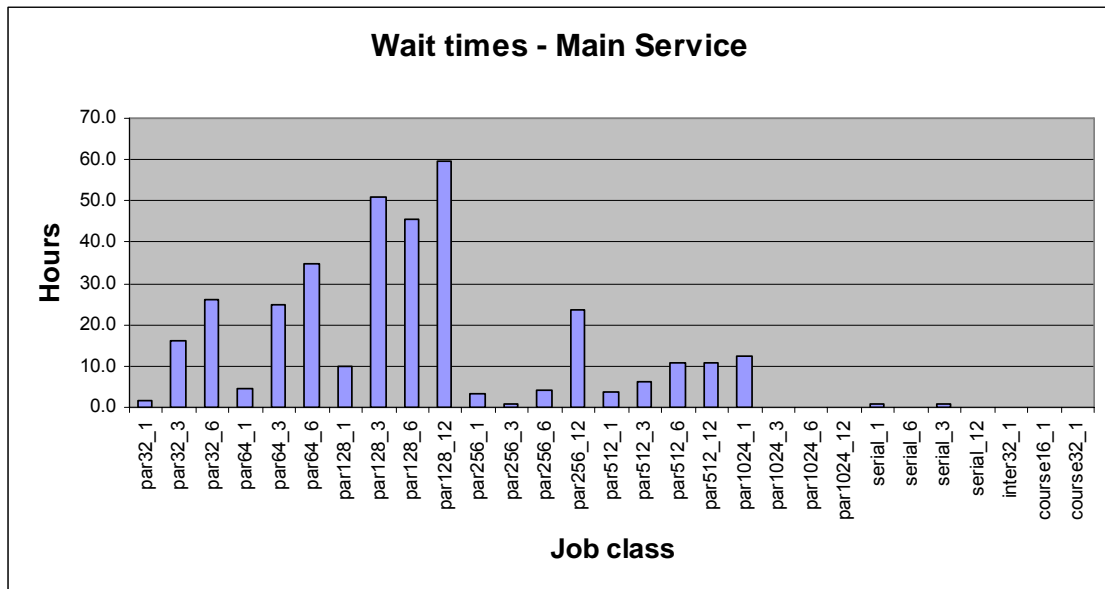


Job wait times

The following table and graph shows the average wait time (in hours) for each class of job on the main service. Wait times were in general satisfactory. Long wait times for the longer 128-processor continue to be significant; we have taken this into account in planning the configuration for the Phase 3 system, which will have a much larger capability region.

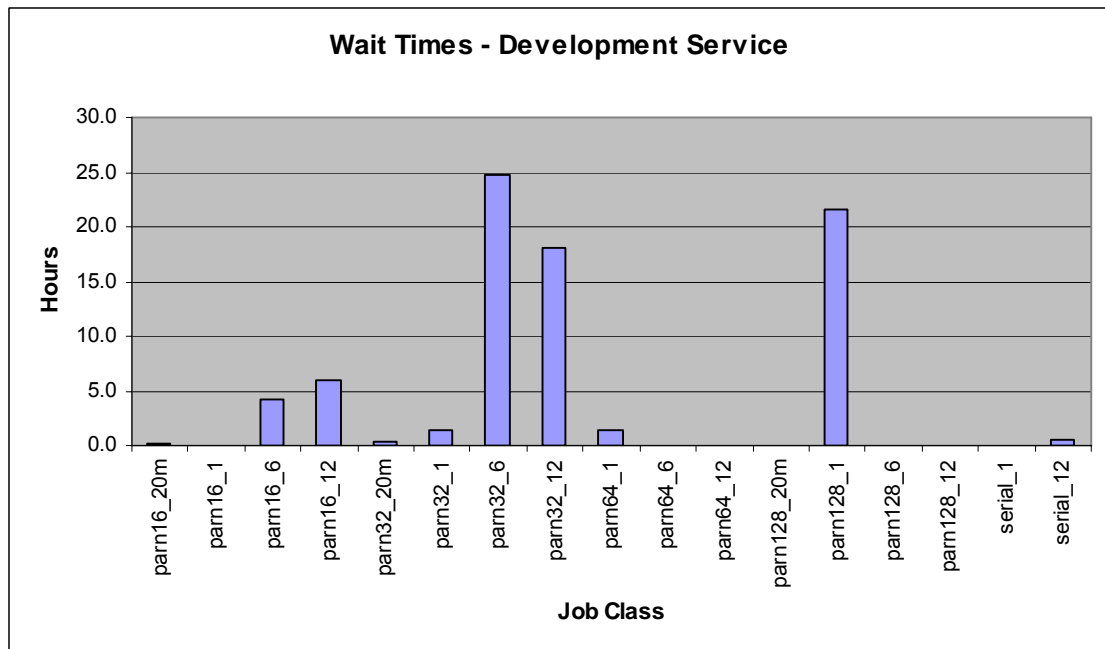
Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	parallel	32	1	1.5	1862
par32_3	parallel	32	3	16.3	170
par32_6	parallel	32	6	26.3	480
par64_1	parallel	64	1	4.7	378
par64_3	parallel	64	3	24.8	32
par64_6	parallel	64	6	34.7	151
par128_1	parallel	128	1	9.8	166
par128_3	parallel	128	3	50.8	34
par128_6	parallel	128	6	45.5	53
par128_12	parallel	128	12	59.6	128
par256_1	parallel	256	1	3.4	410
par256_3	parallel	256	3	0.8	53
par256_6	parallel	256	6	4.2	56
par256_12	parallel	256	12	23.7	164
par512_1	parallel	512	1	3.7	55
par512_3	parallel	512	3	6.4	20
par512_6	parallel	512	6	10.8	4
par512_12	parallel	512	12	10.8	46
par1024_1	parallel	1024	1	12.6	27

par1024_3	parallel	1024	3	0.0	0
par1024_6	parallel	1024	6	0.0	0
par1024_12	parallel	1024	12	0.0	0
serial_1	serial	1	1	0.9	668
serial_6	serial	1	6	0.0	47
serial_3	serial	1	3	0.9	21
serial_12	serial	1	12	0.2	67
inter32_1	interactive	32	1	0.0	4360
course16_1	interactive	16	1	0.0	18
course32_1	parallel	32	1	0.0	0



The wait times for the development service are shown below.

<i>Job Class</i>	<i>Category</i>	<i>Maximum Number of CPUs</i>	<i>Maximum Job length</i>	<i>Average wait time</i>	<i>Number of Jobs</i>
parn16_20m	parallel	16	20 mins	0.1	670
parn16_1	parallel	16	1 hour	0.1	1163
parn16_6	parallel	16	6 hours	4.2	151
parn16_12	parallel	16	12 hours	5.9	186
parn32_20m	parallel	32	20 mins	0.3	299
parn32_1	parallel	32	1 hour	1.5	422
parn32_6	parallel	32	6 hours	24.7	136
parn32_12	parallel	32	12 hours	18.1	324
parn64_1	parallel	64	1 hour	1.4	1043
parn64_6	parallel	64	6 hours	0.0	0
parn64_12	parallel	64	12 hours	0.0	0
parn128_20m	parallel	128	20 mins	0.0	0
parn128_1	parallel	128	1 hour	21.6	27
parn128_6	parallel	128	6 hours	0.0	0
parn128_12	parallel	128	12 hours	0.0	0
serial_1	serial	1	1 hour	0.1	3160
serial_12	serial	1	12 hours	0.5	15



2.5 Disk Occupancy

Home Space

Home space is the part of the disk space that is regularly backed up.

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
b02	34,058.1	50,000
b03	52,710.5	50,000
b08	937.0	50,000
c01	125,261.8	150,000
e01	58,827.2	58,829
e02	23,079.3	38,829
e03	78,486.0	225,012
e05	241,603.7	450,500
e06	259,586.6	300,000
e08	54,656.9	100,000
e10	74,275.3	150,000
e11	37,017.5	100,000
e14	86,948.6	100,000
e15	34,681.2	50,000
e16	132.9	20,000
e17	44,459.5	50,000
e18	27,399.1	40,000
e19	1,408.2	40,000
e20	58,508.3	60,000
e21	488.3	50,000
e22	993.1	10,000
e23	24.1	50,000
e24	64,696.6	200,000
e25	9,318.0	50,000
e26	13,933.9	20,000
e27	8,225.0	20,000
e29	20,835.3	30,000
e30	0.1	40,000
e31	40,978.2	50,000
e32	47,038.4	50,000
e33	1,224.0	50,000
e34	0.1	50,000
e35	3,939.1	100,000
e36	39,020.7	50,000
e37	83,100.5	100,000
e38	3,346.9	50,000
e39	5,757.2	50,000
e40	5,016.9	50,000

e41	1,521.2	100,000
e42	96,652.7	100,000
e45	6,811.6	50,000
e46	0.1	50,000
e47	0.1	50,000
e48	4.8	50,000
e49	9,060.9	50,000
e50	1,154.4	13,000
e51	2,148.3	50,000
e52	0.4	50,000
e53	1,158.0	50,000
e54	12.2	50,000
e55	0.3	50,000
e56	11,493.0	50,000
n01	46,083.0	100,000
n02	104,315.7	228,000
n03	59,298.3	100,000
n04	298,079.4	299,999
p01	131,688.9	200,000
x01	39,822.4	50,000
x02	8,746.2	20,000
x03	634.8	50,000
z001	285,875.8	320,001
z002	32,016.0	48,001
z003	0.2	3
z004	78,767.7	100,000
z05	4,188.4	30,000
z06	49,752.6	50,000
z07	27,848.8	50,000

Workspace

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
b02	14.8	1,025
b03	47,907.9	100,000
b08	5,019.6	50,000
c01	87,830.2	100,000
e01	1,058,636.2	1,249,995
e02	8,354.8	10,000
e03	9.8	500,000
e05	235,267.6	498,004
e06	271,778.9	400,000
e08	140.8	5,000
e10	284,222.9	400,000
e11	31,947.2	100,000
e14	151,485.7	200,000

e15	34,684.8	100,000
e16	0.2	60,000
e17	2,122.1	100,000
e18	24,819.6	80,000
e19	169,044.5	200,000
e20	931,178.7	1,000,000
e21	1.2	100,000
e22	0.1	20,000
e23	0.1	100,000
e24	570,245.9	750,000
e25	121,934.7	150,000
e26	0.1	40,000
e27	0.4	40,000
e29	5,296.1	8,000
e30	0.1	80,000
e31	96,128.1	100,000
e32	90,365.8	100,000
e33	2,221.1	100,000
e34	0.1	100,000
e35	0.2	200,000
e36	0.1	50,000
e37	44,017.8	150,000
e38	0.1	100,000
e39	0.2	100,000
e40	0.3	100,000
e41	5,122.0	200,000
e42	198,856.9	200,000
e45	0.1	100,000
e46	0.1	50,000
e47	0.1	160,000
e48	0.1	200,000
e49	17,410.3	50,000
e50	4,938.3	100,000
e51	0.2	100,000
e52	0.1	50,000
e53	611.4	150,000
e54	0.2	100,000
e55	0.1	100,000
e56	0.1	100,000
n01	235,180.3	800,000
n02	1,594,931.2	2,099,004
n03	21.6	41,002
n04	175,792.8	750,000
p01	41,764.4	50,000
x01	103,218.7	160,000
x02	0.2	20,000
x03	177.7	50,000
z001	359,936.0	399,999

z002	387.6	770
z003	0.2	3
z004	2,037.5	25,000
z05	4,739.7	20,000
z06	72,653.7	100,000
z07	20.0	20,000

Development space

This is the disk space reserved for users of the development service.

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
n01	0.0	500,000
n02	4,130,521.8	5,220,003
n04	358,794.7	526,899

2.6 Tape Archive

Project Code	Usage(Tapes)	Quota(Tapes)	Files	Data(Gb)	Space(Gb)
c01	2	2	7,231	65.1	308
e01	48	50	148,086	4,262.60	854
e03	5	5	18,797	429.2	84
e14	10	10	384,046	603.8	522
e15	1	3	26	6.1	330
e24	10	10	6,802	662	423
e26	2	2	545	26.9	188
e42	5	5	104	136.9	402
n01	218	220	29,034	23,261.20	1,070
n02	298	300	194,218	37,718.40	3,382
n04	28	30	116,775	3,740.10	378
z001	7	10	11,045	66.5	1,120
z002	3	4	5,802	14.6	591
z06	1	3	833	67.9	493

Note that a tape is counted in the *Usage* column even if it is only partly occupied.

3 Support

3.1 Helpdesk

Classifications

<i>Category</i>	<i>Number</i>	<i>% of all</i>
Administrative	41	47.1
Technical	41	47.1
In-depth	4	4.6
PMR	1	1.1
TOTAL	87	100.0

The PMR category indicates in-depth queries that result in Problem Management Reports for IBM.

<i>Service Area</i>	<i>Number</i>	<i>% of all</i>
Phase 2 platform	83	95.4
Website	2	2.3
Other/general	2	2.3
TOTAL	87	100.0

Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	62	75.6	75%
Finished within 72 Hours	79	96.3	97%
Finished after 72 Hours	3	3.7	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	39	95.1	97%
Finished after 48 Hours	2	4.9	

Experts Handling Queries

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	25	11	2	0
dl.ac.uk	4	17	1	0
Sysadm	12	13	1	1
Other people	0	0	0	0

3.2 Training

<i>Title of Course</i>	<i>Start Date</i>	<i>Length (Days)</i>	<i>Place days</i>	<i>HPCx User Days</i>	<i>HPCx Staff Days</i>
Introduction to HPCx	28-Sep	1	14	5	3

4 Staffing

4.1 Science Support Staffing

Daresbury Laboratory

<i>Name</i>	<i>Days</i>
Ashworth	11.5
Blake	2.1
Bush	15.0
Guest	5.3
Johnstone	21.0
Jones	3.7
Plummer	8.5
Sunderland	21.0
Thomas	8.4
Total (Days)	96.5
FTEs	5.4

EPCC

<i>Name</i>	<i>Days</i>
Simpson	16.2
Booth	14.7
Henty	6.9
Smith	11.7
Bull	2.8
Fisher	6.0
Hein	7.6
Jackson	5.0
Pringle	0.7
Reid	8.1
Stratford	1.0
Nazarova	8.8
Trew	4.3
Gray	6.2
D'Mellow	2.6
Hill	0.6

Maynard	5.8
Other staff	38.7
Helpdesk	0.9
Total (Days)	148.4
FTEs	8.4

Overall Levels

	<i>FTEs</i>
DL	5.4
EPCC	8.4
Total	13.8

4.2 Systems Staffing

<i>Name</i>	<i>Days</i>
Andrews	15.8
Blake	0.0
Brown	21.0
Fisher	6.0
Georgeson	15.8
Franks	15.0
Jones	0.9
Shore	15.8
BITD	16.8
Total (Days)	107.0
FTEs	6.0

Note: BITD covers a range of bookings from a support department who provide approximately 1 FTE to support computer room operations, electrical and mechanical site services and networking and security. Roughly a dozen staff charge time to the project in amounts which vary from month to month. We believe that it adds no value to report these individual bookings although a full listing can be provided annually if required.

5 Summary of Performance Metrics

<i>Metric</i>	<i>TSL</i>	<i>FSL</i>	<i>Monthly Measurement</i>
Technology serviceability	80%	99.2%	100.0%
Technology MTBF (hours)	200	300	∞
Number of AV FTEs	7.5	10	13.8
Number of training days per month	20/12	25/12	22/9
Non in-depth queries resolved within 3 days	85%	97%	96.3%
Number of A&M FTEs	3.75	5.75	6.0
A&M serviceability	80%	99.6%	99.4%

Appendix A: 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 filesystems 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

B.1 Current Projects

EPSRC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
e01	1	UK Trubulence Consortium	Dr Gary Coleman
e05	1	Materials Chemistry using Terascaling Computing	Prof Richard Catlow
e06	1	UK Car-Parrinello Consortium	Prof Paul Madden
e07	2	Turbulent Plasma Transport in Tokamaks	Dr Colin M Roach
e08	2	Organic Solid State	Prof Sarah Price
e10	1	Reality Grid	Prof Peter Coveney
e11	1	Bond making and breaking at surfaces	Prof Sir David A King
e14	1	Blade and Cavity Noise	Prof Neil Sandham
e15	2	CSAR/HPCx Collaboration	Dr Mike Pettipher
e16	1	Cardiac virtual tissues	Prof Arun V Holden
e17	1	Integrative Biology	Dr David Gavaghan
e18	1	DARP: Highly swept leading edge separations	Prof Michael A Leschziner
e19	1	Edinburgh Soft Matter and Statistical Physics Group	Prof Michael E Cates
e20	1	UK Applied Aerodynamics Consortium	Dr Ken Badcock
e21	1	Intrinsic Parameter Fluctuations in Decanometer MOSFETs	Prof Asen M Asenov
e22	1	Preconditioners for finite element problems	Prof David J Silvester
e23	1	Exploitation of Switched Lightpaths for e-Science Applications	Prof Peter Clarke
e24	1	DEISA - Distributed European Infrastructure for Supercomputing Applications	Dr David Henty
e25	1	Turbulent vortex motion in stratified flows	Dr Gary Coleman
e26	1	Simulation of Radioprobing	Dr Charlie Laughton
e27	1	SPICE	Prof Peter V Coveney

e29	1	Free-surface-piercing circular cylinders	Dr Eldad Avital
e30	1	Metal/Oxide Interfaces at the Atomic Level	Dr Nora de Leeuw
e31	1	Lateral Straining of Wall-Bounded Turbulence	Dr Gary N Coleman
e32	1	Rapid Prototyping of Usable Grid Middleware	Prof Peter V Coveney
e33	1	Engineering Functional Coatings	Prof Roger Smith
e34	1	Dissolution of Bioactive Phosphate Glasses	Dr N de Leeuw
e35	1	Non-adiabatic processes	Dr T Todorov
e36	1	Jets in Cross-Flow	Dr Y Yao
e37	1	LESUK_3	Prof J J McQuirk
e38	1	Viscoelastic deformation in 3D non-linear media	Prof Greg A Houseman
e39	1	The Supergen 5 biological fuel cells consortium	Prof FA Armstrong
e40	1	Computational Quantum Many-Body Theory	Prof R Needs
e41	1	Flow in Weapon Bays	Dr George N Barakos
e42	1	Computational Combustion for Engineering Applications	Prof K Luo
e45	1	Metals under extreme conditions	Prof Mike Gillan
e46	1	Advanced materials with complex architectures	Dr Paul Mummery
e47	1	Parallel stochastic analysis for geo-engineering	Dr Michael A. Hicks
e48	1	Organised structure in turbulent flows	Prof Sergei Chernyshenko
e49	1	Integrated Programme of Research in Aeronautical Engineering	Prof Michael Leschziner
e50	1	Biological interface with materials	Prof John Harding
e51	1	Super-computing data mining	Dr Mike Pettipher
e52	1	Spacecraft force modelling	Dr M Ziebart
e53	1	Large-scale communication networks	Prof J M Pitts
e54	1	Free surface simulation of waves overtopping during storms	Dr D M Ingram
e55	1	High-Reynolds-Number Near-Wall Flows	Prof Michael Leschziner
e56	1	Infectious disease threats	Dr Iain Barrass
z09		HECToR Benchmarking	Dr Edward Smyth

Note: The original project e01 ended on 30 April 2005. The new UKTC project started on 1 March 2006. At the request of the PI it was assigned the same code as the old one, and inherited its disk space.

PPARC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
p01	1	Atomic Physics and Astrophysics	Prof Alan Hibbert

NERC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
n01	1	Large-Scale Long-Term Ocean Circulation	Dr David Webb
n02	1	NCAS	Prof Alan J Thorpe
n03	1	Computational Mineral Physics Consortium	Dr John Brodholt
n04	1	Shelf Seas Consortium	Dr Roger Proctor

BBSRC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
b02	1	Modelling enzyme catalysis	Dr Adrian J Mulholland
b08	1	IntBioSim	Prof M S Sansom

CCLRC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
c01	1	Daresbury Laboratory Facilities Agreement Consortium	Dr Richard J Blake

Externally-funded Projects

<i>Code</i>	<i>Title</i>	<i>PI</i>
x01	HPC-Europa	Dr J-C Desplat
x03	IBM	Mr Derrick J Byford

HPCx Projects

<i>Code</i>	<i>Title</i>	<i>PI</i>
z001	HPCx Support	Dr Alan Simpson
z002	Systems and Operations	Mr Mike Brown
z003	Test Project	Dr Denis Nicole
z004	HPCx Training	Dr David Henty
z05	Outreach Projects	Dr Richard Blake
z06	Application Porting	Dr David Henty
z07	Package Installation	Dr Mike Ashworth

B.2 Former Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
b01	2	Quantum Chemistry Studies of the Rusticyanin Protein Crystal	Prof Samar Hasnain
b03	1	Towards a virtual outer membrane	Prof Mark S Sansom
b04	1	Life sciences software development	Dr Jo L Dicks
b05	1	Virtual forced evolution of catalytic transition metal complexes	Dr Marcus Durrant
b06	2	Biomolecular computational chemistry	Prof Jonathan D Hirst
e02	1	Ab-initio simulation of covalently bonded materials	Dr Patrick Briddon
e03	1	Multi-photon, electron collisions and BEC HPC consortium	Prof Ken Taylor
e04	1	Chemreact Computing Consortium	Prof Jonathon Tennyson
e07	2	Turbulent Plasma Transport in Tokamaks	Dr Colin M Roach
e09	2	Molecular Properties and their Geometry	Dr Mark R Wilson
e12	1	Parallel programs for the simulation of complex fluids	Dr Richard J Blake
e13	1	TeraGyroid project	Mr Mark Westwood
e28	1	Towards the Dynome	Dr Jonathan W Essex
z09		HECToR Benchmarking	Dr Edward Smyth
x02		OHM Ltd	Dr Lucy MacGregor
n05	2	Non-linear Wave-particle Instabilities in Plasmas	Dr Mervyn Freeman