

HPCx Service Report October 2006

1 Introduction

This report covers the period from 0800 on 1 October 2006 to 0800 on 1 November 2006. Taking into account the end of summer time, this was a service month of 745 hours.

Phase 3 of HPCx started on October 5. Acceptance tests were run successfully over 16-17 October, and the ten-day reliability test was completed before the end of the month. Despite this large increase in available time, utilisation of the main service for the whole month reached 74.5%. Capability use was 36.5% of the total.

2 Usage

2.1 Availability

Incidents

During this month, there were 13 incidents, two of which were 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	2
2	1
3	9
4	1

The MTBF figures for this month were as follows:

<i>SEV1</i>	<i>Incidents</i>	<i>MTBF</i>
IBM	1.0	720
Site	0.0	∞
External	1.0	720
<i>Overall</i>	2.0	360

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>
06.095	0%	100%	0%	Maintenance session overrun
06.106	0%	0%	100%	Loss of external network

Serviceability

Scheduled downtime for this month was 56.3 hours. This included time required to prepare for the change to Phase 3, and the Phase 3 acceptance trials.

<i>Attribution</i>	<i>UDT</i>	<i>Serviceability</i>
IBM	1:20	99.8
Site	0:00	100.0
External	0:20	99.9
<i>Overall</i>	1:40	99.8

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	45463	256	220112	3.9%
e03	333	0	1605	0.0%
e05	191363	527	903926	16.2%
e06	7710	249	38319	0.7%
e08	32364	0	155813	2.8%
e14	291	12	1462	0.0%
e15	644	0	3100	0.1%
e17	9299	0	44767	0.8%
e18	0	0	0	0.0%
e19	61	0	296	0.0%
e20	41263	0	198658	3.6%
e22	0	0	0	0.0%
e23	5	0	24	0.0%
e24	91387	0	439978	7.9%
e25	0	4	17	0.0%
e26	1597	0	7690	0.1%
e27	487	0	2342	0.0%
e33	44968	0	216494	3.9%
e35	11712	73	56740	1.0%
e36	6742	3	32473	0.6%
e37	23039	12	110976	2.0%
e38	14	0	68	0.0%
e39	17194	0	82782	1.5%
e40	1	0	7	0.0%
e42	260166	56	1252828	22.4%
e45	3107	0	14959	0.3%
e48	1972	1	9501	0.2%
e49	3552	1	17104	0.3%
e50	4741	0	22827	0.4%
e51	1	0	4	0.0%
e53	320	0	1541	0.0%
e54	166	0	801	0.0%
e56	4764	0	22934	0.4%
<i>EPSRC Total</i>	804728	1194	3860148	69.1%

n01	123827	25	596281	10.7%
n02	31770	2	152964	2.7%
n03	80333	0	386760	6.9%
n04	9906	0	47692	0.9%
<i>NERC Total</i>	245836	27	1183698	21.2%

p01	7137	1	34363	0.6%
<i>PPARC Total</i>	7137	1	34363	0.6%

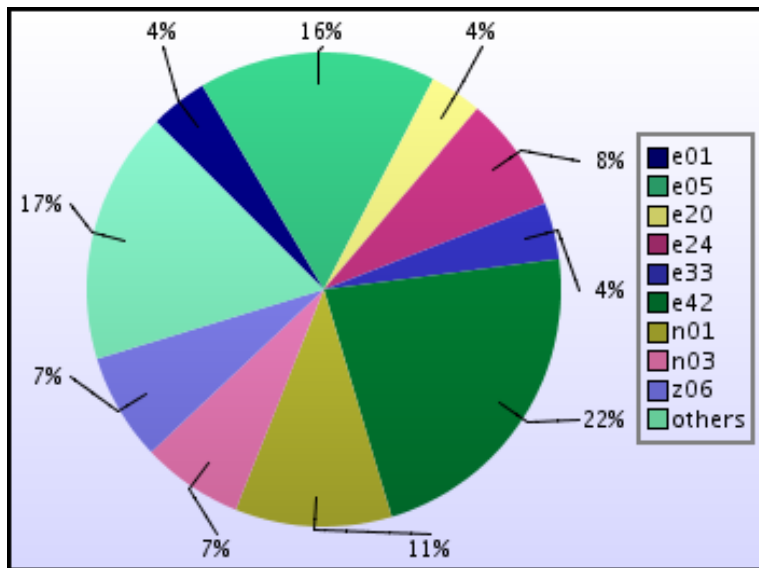
c01	2554	31	12444	0.2%
<i>CCLRC Total</i>	2554	31	12444	0.2%

b08	2057	15	9974	0.2%
<i>BBSRC Total</i>	2057	15	9974	0.2%

x01	2377	49	11677	0.2%
<i>External Total</i>	2377	49	11677	0.2%

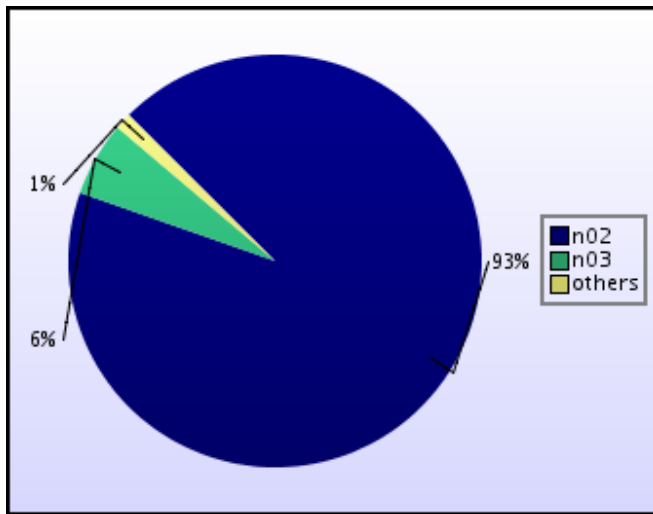
z001	13117	3	63166	1.1%
z002	0	0	0	0.0%
z004	262	1	1267	0.0%
z06	84511	0	406874	7.3%
<i>HPCx Total</i>	97890	4	471306	8.4%

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	0	0	0	0.0%
n02	103186	180	497648	92.9%
n03	6500	0	31294	5.8%
n04	1453	0	6994	1.3%
<i>NERC Total</i>	<i>111138</i>	<i>180</i>	<i>535937</i>	<i>100.0%</i>



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	479627	8.6%	3429
33–64	478732	8.6%	794
65–128	1124828	20.1%	574
129–256	1470567	26.3%	434
257–512	503088	9.0%	119
513–1024	1139745	20.4%	52
>1024	400588	7.2%	17

Utilisation by region

The regions of the main service under Phase 2A were:

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

Under Phase 3, they are:

- Capacity Region (50 nodes, for jobs using ≤128 CPUs)
- Capability Region (96 nodes, principally for jobs using >128 CPUs)
- Interactive-parallel Region (2 nodes)

As a result of the changes in the sizes of the regions this month, it is difficult to assess the utilisation for each region. Overall utilisation, taking into account the advent of Phase 3, was 74.5%.

Development Service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	463051	86.5%	4671
33–64	34013	6.4%	231
65–128	38006	7.1%	93
129–256	0	0.0%	0

Overall utilisation was 84.1%.

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:

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

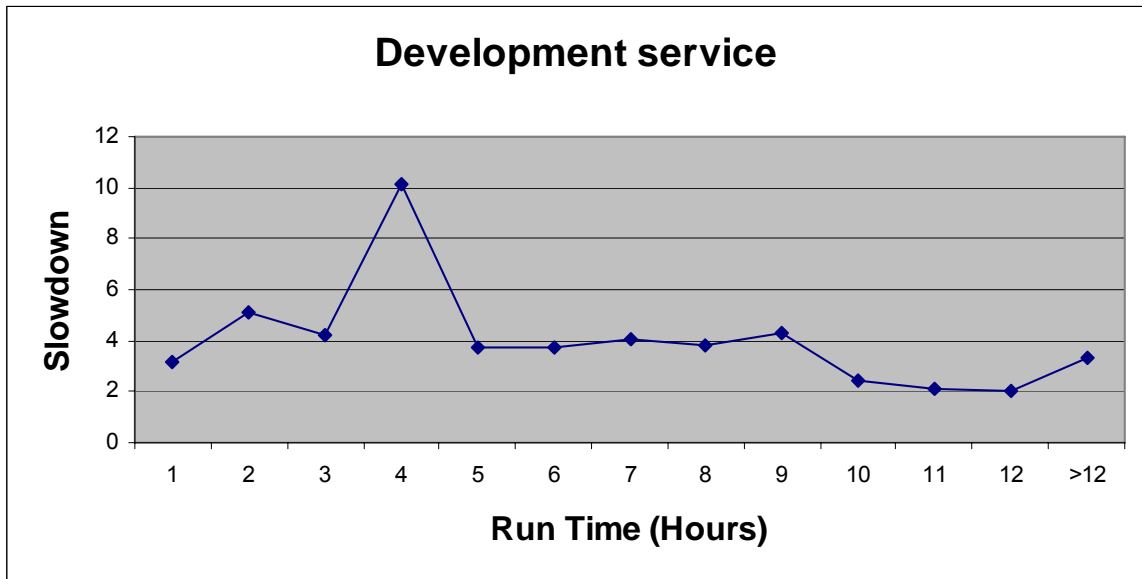
Slowdowns of less than around 10 are usually regarded as reasonable.

On both services, slowdowns are currently satisfactory.

Slowdowns by runtime

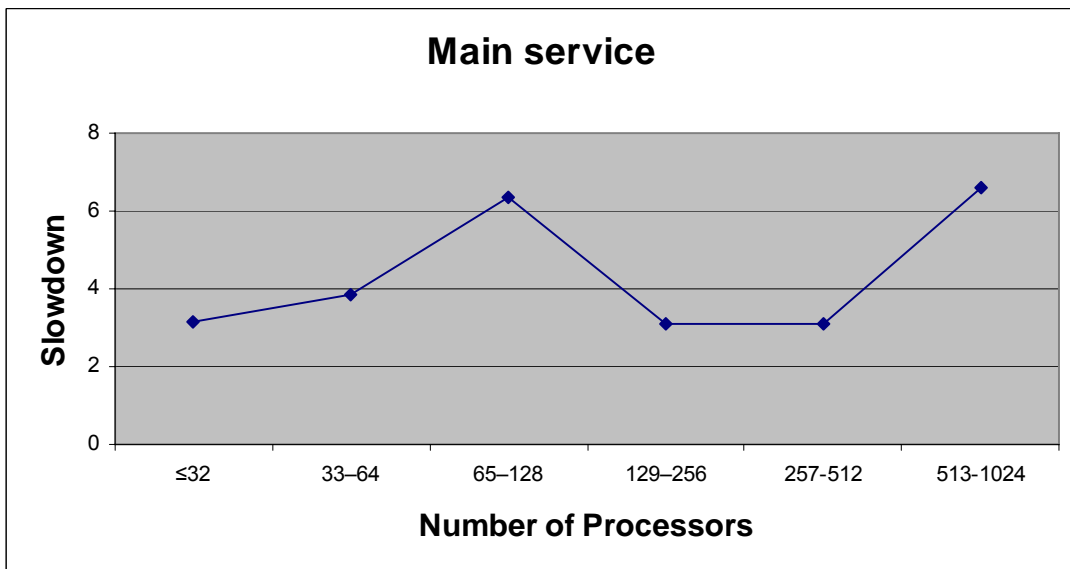
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

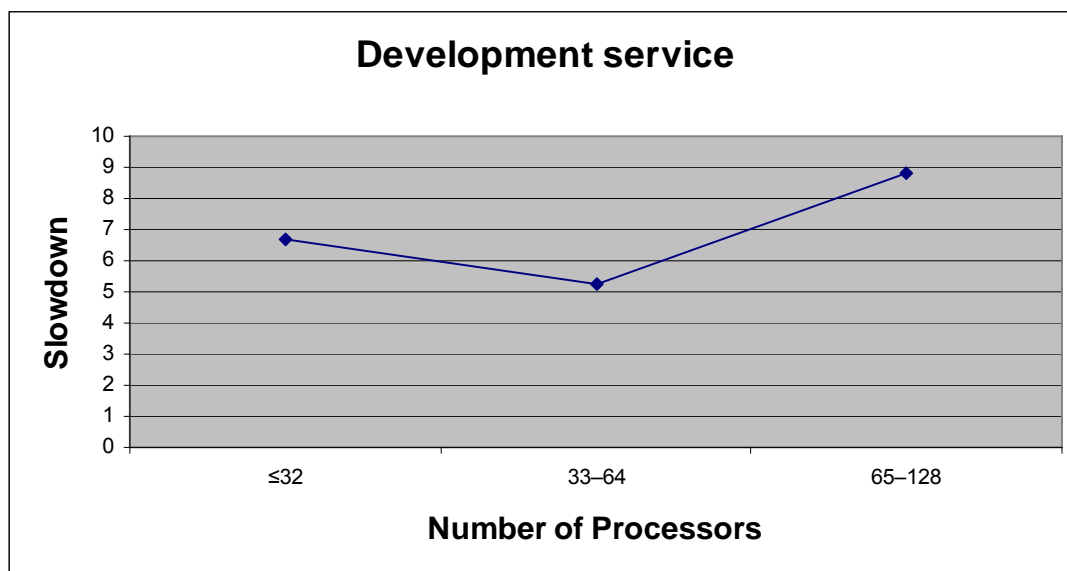




Slowdowns by number of processors

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.



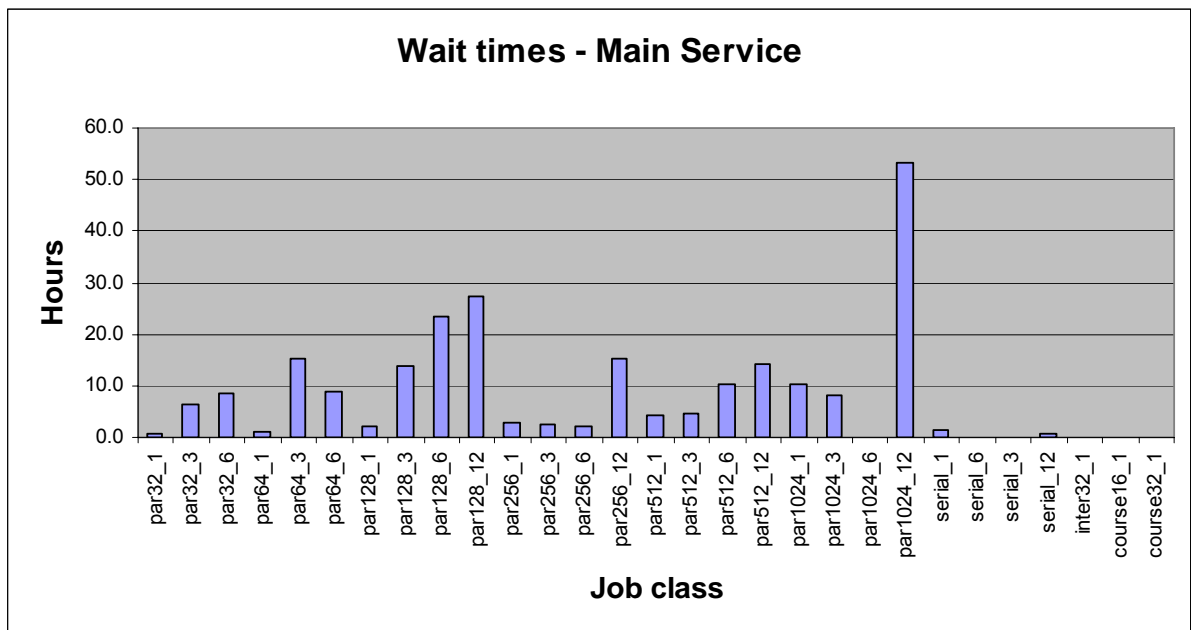


Job wait times

The following table and graph shows the average wait time (in hours) for each class of job on the main service. The long wait times for 1024-processor 12-hour jobs result from the submission of sequences of dependent jobs; for these, the wait time of each job is calculated from the time of the submission of the whole series. The 30 jobs in this class included six sequences of four jobs each.

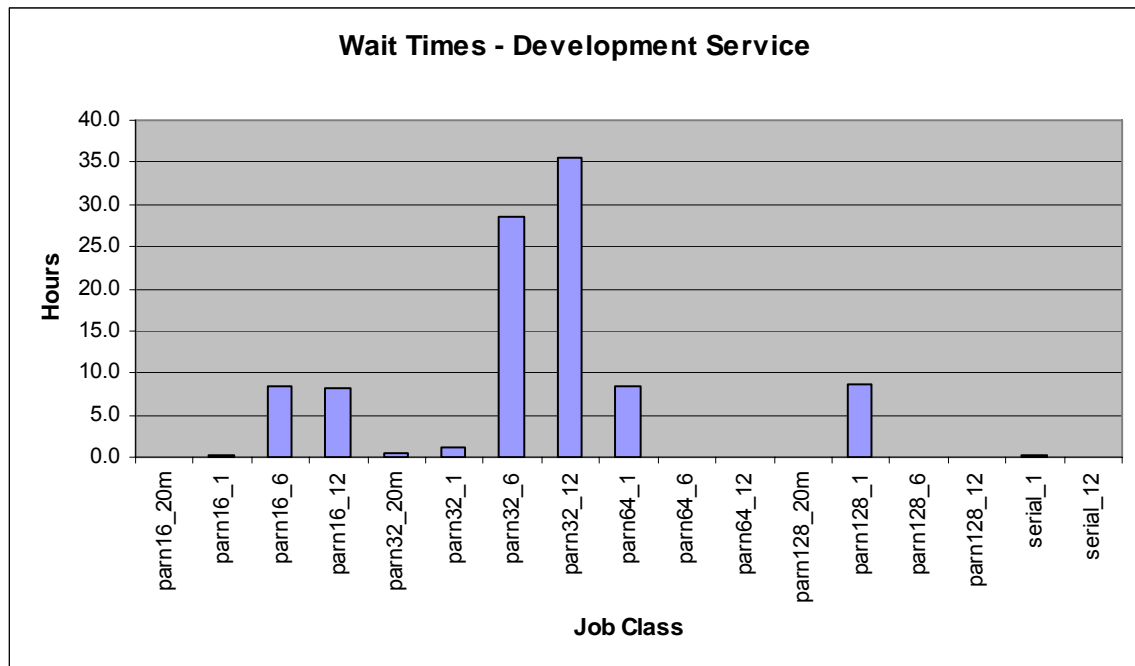
Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	parallel	32	1	0.7	2634
par32_3	parallel	32	3	6.4	92
par32_6	parallel	32	6	8.5	699
par64_1	parallel	64	1	1.0	421
par64_3	parallel	64	3	15.1	74
par64_6	parallel	64	6	9.0	299
par128_1	parallel	128	1	2.1	237
par128_3	parallel	128	3	13.8	89
par128_6	parallel	128	6	23.6	62
par128_12	parallel	128	12	27.4	186
par256_1	parallel	256	1	2.8	194
par256_3	parallel	256	3	2.4	34
par256_6	parallel	256	6	2.2	57
par256_12	parallel	256	12	15.3	149
par512_1	parallel	512	1	4.1	77
par512_3	parallel	512	3	4.5	15
par512_6	parallel	512	6	10.2	7
par512_12	parallel	512	12	14.4	20

par1024_1	parallel	1024	1	10.3	20
par1024_3	parallel	1024	3	8.1	2
par1024_6	parallel	1024	6	0.0	0
par1024_12	parallel	1024	12	53.4	30
serial_1	serial	1	1	1.5	792
serial_6	serial	1	6	0.0	33
serial_3	serial	1	3	0.0	43
serial_12	serial	1	12	0.6	14
inter32_1	interactive	32	1	0.0	4470
course16_1	interactive	16	1	0.0	0
course32_1	parallel	32	1	0.0	0



The wait times for the development service are shown below.

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
parn16_20m	parallel	16	20 mins	0.1	1077
parn16_1	parallel	16	1 hour	0.2	1368
parn16_6	parallel	16	6 hours	8.4	97
parn16_12	parallel	16	12 hours	8.1	198
parn32_20m	parallel	32	20 mins	0.4	350
parn32_1	parallel	32	1 hour	1.1	1257
parn32_6	parallel	32	6 hours	28.5	221
parn32_12	parallel	32	12 hours	35.5	103
parn64_1	parallel	64	1 hour	8.4	157
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	8.7	93
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	3679
serial_12	serial	1	12 hours	0.0	9



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	50,000
b03	52,711	50,000
b08	1,957	50,000
c01	141,639	150,000
e01	46,171	58,829
e02	23,079	38,829
e03	66,152	225,012
e05	284,771	500,500
e06	273,972	300,000
e08	67,562	100,000
e10	74,267	150,000
e11	37,018	100,000
e14	92,678	100,000
e15	35,493	50,000
e16	133	20,000
e17	48,095	50,000
e18	27,454	40,000
e19	1,417	40,000
e20	59,001	60,000
e21	488	50,000
e22	1,184	10,000
e23	26,412	50,000
e24	73,254	365,000
e25	9,406	50,000
e26	16,055	20,000
e27	16,675	20,000
e29	20,835	30,000
e30	0	40,000
e31	40,978	50,000
e32	47,038	50,000
e33	2,995	50,000
e34	0	50,000
e35	14,886	100,000
e36	48,174	50,000
e37	75,745	100,000
e38	7,213	50,000
e39	4,520	50,000
e40	5,923	50,000

e41	1,521	100,000
e42	17,390	100,000
e45	12,720	50,000
e46	0	50,000
e47	0	50,000
e48	5	50,000
e49	36,944	50,000
e50	1,302	13,000
e51	3,305	50,000
e52	11	50,000
e53	1,397	50,000
e54	612	50,000
e55	0	50,000
e56	47,509	50,000
e57	0	50,000
n01	47,833	100,000
n02	165,879	298,000
n03	54,296	100,000
n04	287,027	299,999
p01	176,915	200,000
x01	45,054	50,000
x02	8,746	20,000
x03	4,227	50,000
z001	283,501	400,001
z002	57,979	124,000
z003	0	3
z004	77,847	100,000
z05	4,188	30,000
z06	51,067	75,000
z07	28,516	50,000

Workspace

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
b02	15	1,025
b03	47,908	100,000
b08	5,078	50,000
c01	92,785	100,000
e01	1,088,505	1,249,995
e02	8,355	10,000
e03	10	500,000
e05	238,339	498,004
e06	306,658	400,000
e08	141	5,000
e10	284,223	400,000
e11	37,638	100,000
e14	185,379	200,000

e15	37,318	100,000
e16	0	60,000
e17	4,657	100,000
e18	24,820	80,000
e19	174,172	200,000
e20	931,694	1,000,000
e21	1	100,000
e22	0	20,000
e23	0	100,000
e24	948,551	2,828,999
e25	127,303	150,000
e26	0	40,000
e27	1	40,000
e29	5,296	8,000
e30	0	80,000
e31	96,129	100,000
e32	90,366	100,000
e33	5,622	100,000
e34	0	100,000
e35	0	200,000
e36	1,361	50,000
e37	74,761	150,000
e38	0	100,000
e39	0	100,000
e40	0	100,000
e41	5,122	200,000
e42	202,931	300,000
e45	0	100,000
e46	0	50,000
e47	0	160,000
e48	6,785	200,000
e49	22,828	50,000
e50	8,999	100,000
e51	0	100,000
e52	0	50,000
e53	1,632	150,000
e54	0	100,000
e55	0	100,000
e56	99,999	100,000
e57	0	100,000
n01	321,096	800,000
n02	1,852,483	2,099,004
n03	492	41,002
n04	226,059	750,000
p01	41,764	50,000
x01	121,607	160,000
x02	0	20,000
x03	178	50,000

z001	362,419	500,000
z002	901	770
z003	0	3
z004	4,336	25,000
z05	4,740	20,000
z06	47,680	100,000
z07	21	20,000

Development service 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	500,000
n02	4,789,643.30	6,920,003
n04	242,725	526,899

2.6 Tape Archive

<i>Consortium</i>	<i>Usage (Tapes)</i>	<i>Quota (Tapes)</i>	<i>Files</i>	<i>Data (Gb)</i>
c01	2	2	7231	65
e01	50	50	148470	4541
e03	5	5	18797	429
e14	10	10	384046	604
e15	1	3	26	6
e24	10	10	14952	1790
e26	2	2	545	27
e42	5	5	199	217
n01	225	230	29566	24380
n02	305	310	234560	39696
n04	28	30	116775	3740
z001	7	10	11045	67
z002	3	4	5802	15
z06	1	3	833	68

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	32	40.5
Technical	39	49.4
In-depth	7	8.9
PMR	1	1.3
TOTAL	79	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	72	91.1
Website	5	6.3
Other/general	2	2.5
TOTAL	79	100.0

Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	60	84.5	75%
Finished within 72 Hours	70	98.6	97%
Finished after 72 Hours	1	1.4	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	31	96.9	97%
Finished after 48 Hours	1	3.1	

Experts Handling Queries

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	20	12	5	1
dl.ac.uk	3	13	1	0
Sysadm	9	14	1	0
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>
Application Performance and Tuning Workshop	Oct-12	1	10	7	1

4 Staffing

4.1 Science Support Staffing

Daresbury Laboratory

<i>Name</i>	<i>Days</i>
Ashworth	14.6
Blake	2.1
Bush	19.0
Guest	5.0
Johnstone	21.0
Jones	3.2
Plummer	8.0
Sunderland	16.0
Thomas	8.0
Total (Days)	96.9
FTEs	5.5

EPCC

<i>Name</i>	<i>Days</i>
Simpson	14.5
Booth	11.0
Henty	11.2
Smith	13.7
Bull	3.7
Fisher	4.3
Hein	9.0
Jackson	8.0
Pringle	0.8
Reid	11.5
Stratford	4.4
Nazarova	12.8
Trew	4.3
Gray	15.0
D'Mellow	16.8
Hill	1.7

Johnson	0.3
Maynard	2.6
Other staff	40.3
Helpdesk	0.7
Total (Days)	189.8
FTEs	10.7

Reported under *Other staff* are the additional contributions of recently-graduated MSc students, employed on a temporary basis.

Overall Levels

	<i>FTEs</i>
DL	5.5
EPCC	10.5
Total	16.0

4.2 Systems Staffing

<i>Name</i>	<i>Days</i>
Andrews	16.2
Blake	0.0
Brown	22.0
Fisher	8.7
Georgeson	18.9
Franks	14.4
Jones	0.8
Shore	4.8
BITD	16.8
Total (days)	102.6
FTEs	5.8

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%	99.8%
Technology MTBF (hours)	200	300	720
Number of AV FTEs	7.5	10	16.0
Number of training days per month	20/12	25/12	23/10
Non in-depth queries resolved within 3 days	85%	97%	98.6%
Number of A&M FTEs	3.75	5.75	5.8
A&M serviceability	80%	99.6%	100.0%

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 Turbulence 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 McGuirk
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

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 Judy Hardy
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