

HPCx Service Report

August 2006

1 Introduction

This report covers the period from 1 August 2006 at 0800 to 1 September 2006 at 0800, a service month of 744 hours.

Utilisation of the main service has now returned to typical levels, exceeding 80% for the first time since March. Capability use was nearly 40% of the total, the highest value this year. The two largest user projects were n02 (NCAS), with more than 800,000 AUs on the two services, and e42 (the new Computational Combustion project of Prof Kai Luo) with more than 700,000 AUs.

2 Usage

2.1 Availability

Incidents

During this month, there were 13 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	3
3	9
4	0

The MTBF figures for this month were as follows:

<i>SEV1</i>	<i>Incidents</i>	<i>MTBF</i>
IBM	1.0	732
Site	0.0	∞
External	0.0	∞
<i>Overall</i>	1.0	732

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>
06.078	0%	100%	0%	GPFS failure

Serviceability

Scheduled downtime for this month was 18.7 hours.

<i>Attribution</i>	<i>UDT</i>	<i>Serviceability</i>
IBM	11:17	98.4
Site	0:00	100.0
External	0:00	100.0
<i>Overall</i>	11:17	98.4

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	40233	124	194295	4.7%
e03	827	0	3983	0.1%
e05	80075	547	388152	9.4%
e06	16556	297	81136	2.0%
e08	38265	49	184462	4.5%
e11	10326	0	49714	1.2%
e14	73343	14	353174	8.5%
e15	460	3	2226	0.1%
e17	2258	28	11005	0.3%
e18	466	0	2242	0.1%
e20	31765	35	153102	3.7%
e21	0	12	58	0.0%
e24	25077	21	120837	2.9%
e25	37	137	839	0.0%
e27	40105	0	193081	4.7%
e31	147	0	705	0.0%
e33	35075	0	168867	4.1%
e35	100	14	548	0.0%
e36	153	0	735	0.0%
e37	11916	0	57371	1.4%
e38	191	0	917	0.0%
e39	7418	0	35712	0.9%
e40	2901	1	13971	0.3%
e41	599	0	2881	0.1%
e42	145876	29	702453	17.0%
e45	12010	0	57823	1.4%
e49	213	0	1024	0.0%
e50	10936	0	52653	1.3%
e51	97	0	466	0.0%
e53	118	11	620	0.0%
e54	109	71	868	0.0%
e56	1498	0	7214	0.2%
<i>EPSRC Total</i>	589149	1393	2843134	68.8%

n01	90311	24	434914	10.5%
n02	72493	9	349059	8.4%
n03	13630	0	65622	1.6%
n04	49911	28	240425	5.8%
<i>NERC Total</i>	226345	61	1090020	26.4%

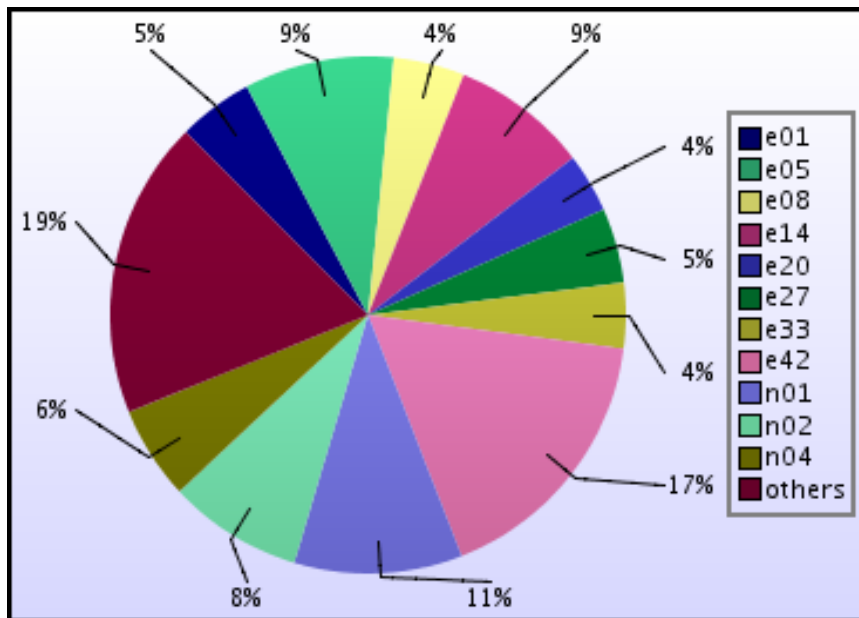
p01	2506	2	12071	0.3%
<i>PPARC Total</i>	2506	2	12071	0.3%

c01	21457	199	104260	2.5%
<i>CCLRC Total</i>	21457	199	104260	2.5%

b08	999	0	4810	0.1%
<i>BBSRC Total</i>	999	0	4810	0.1%

x01	2681	0	12906	0.3%
<i>External Total</i>	2681	0	12906	0.3%

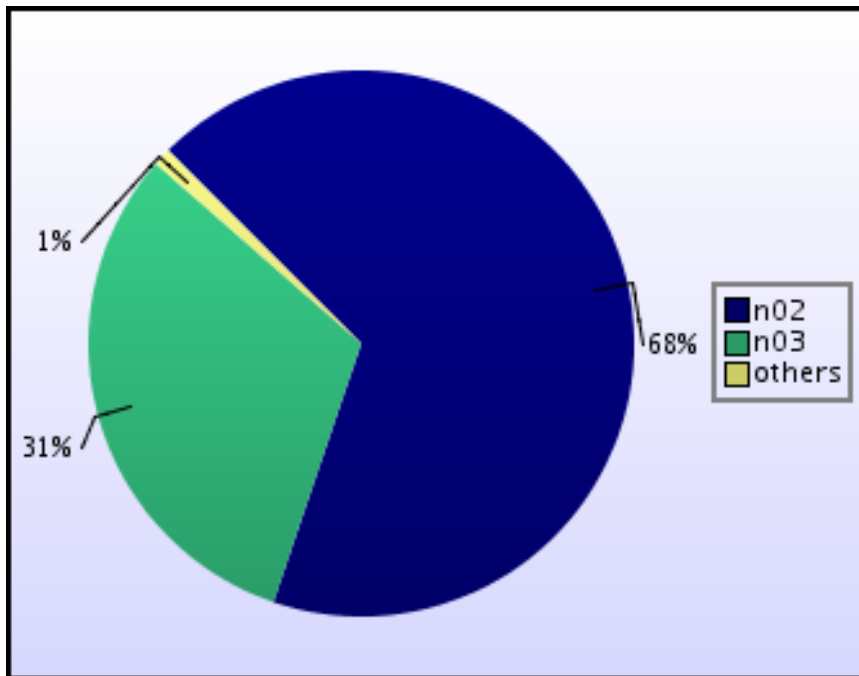
z001	12623	50	61013	1.5%
z002	0	0	1	0.0%
z004	518	43	2701	0.1%
<i>HPCx Total</i>	13141	93	63714	1.5%



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	199	0	958	0.1%
n02	97792	462	473041	67.7%
n03	45284	0	218019	31.2%
n04	1170	0	5633	0.8%
<i>NERC Total</i>	144446	462	697650	99.9%

z001	175	0	843	0.1%
<i>HPCx Total</i>	175	0	843	0.1%



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	426344	10.3%	3251
33–64	320691	7.8%	973
65–128	575200	14.0%	410
129–256	1165185	28.3%	434
257–512	921266	22.3%	111
513–1024	713799	17.3%	54

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 80.2%.

Development Service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	587728	84.4%	5995
33–64	101794	14.6%	558
65–128	6746	1.0%	33
129–256	0	0.0%	0

On 17 August, 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. Consequently an extra 226,780 AUs were available this month, and this resulted in a large increase in the number of AUs used. Overall utilisation of the enlarged development service was 77.6%, equivalent to 103.9% of the normally-available AUs.

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:

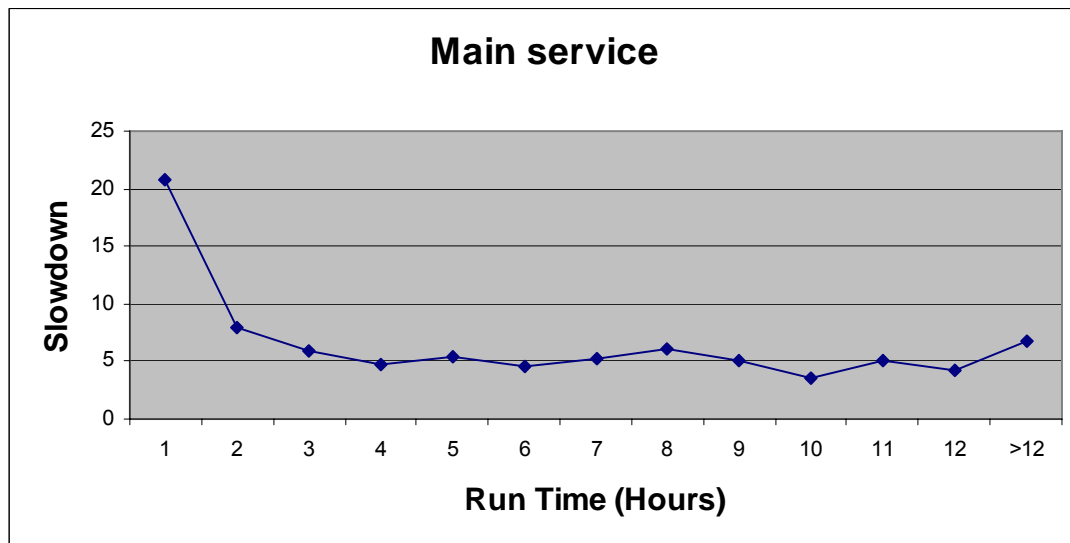
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

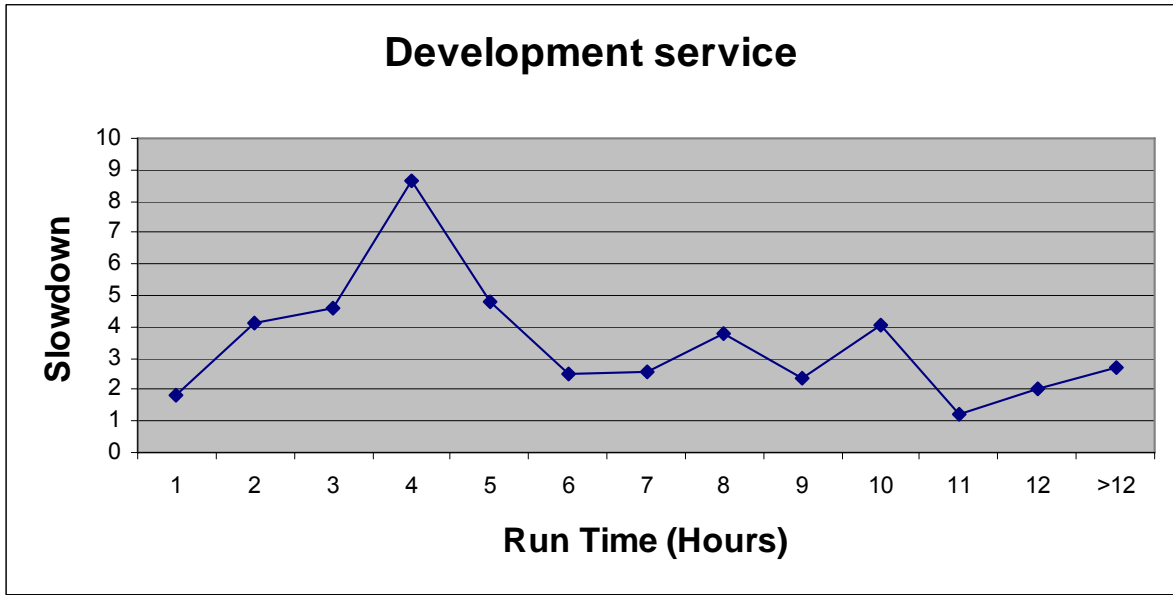
Slowdowns of less than around 10 are usually regarded as reasonable.

On both services, slowdowns are currently satisfactory.

Slowdowns by runtime

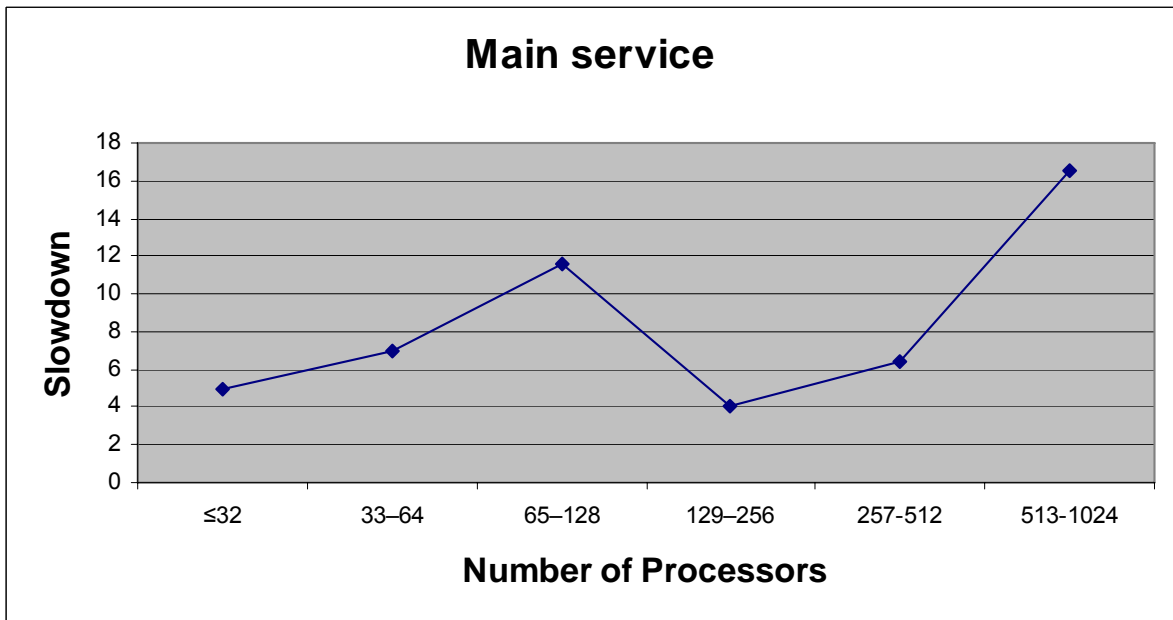
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

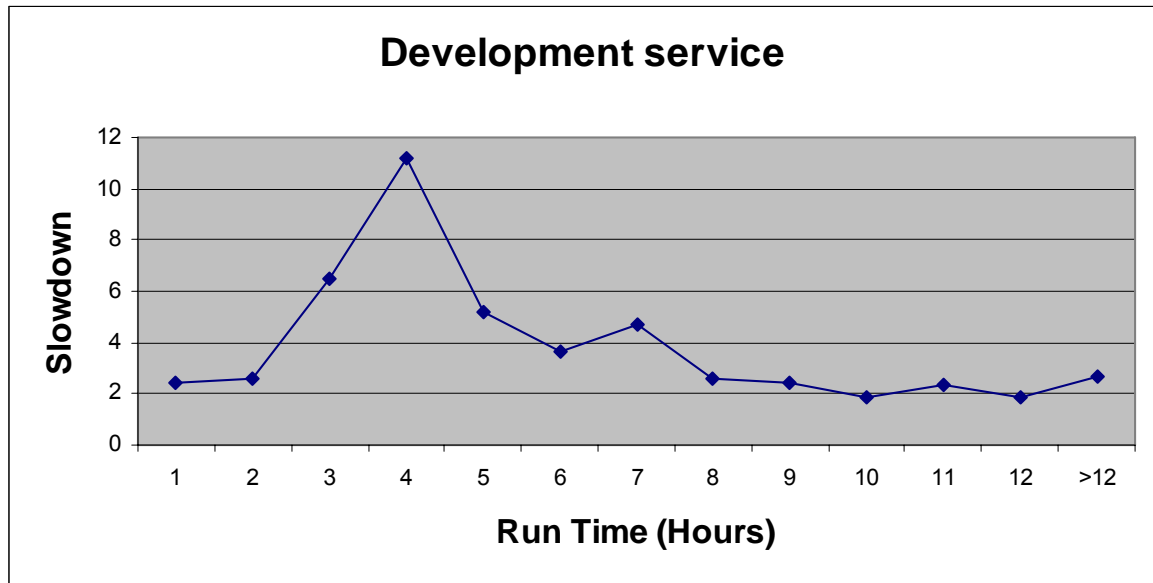




Slowdowns by number of processors

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.



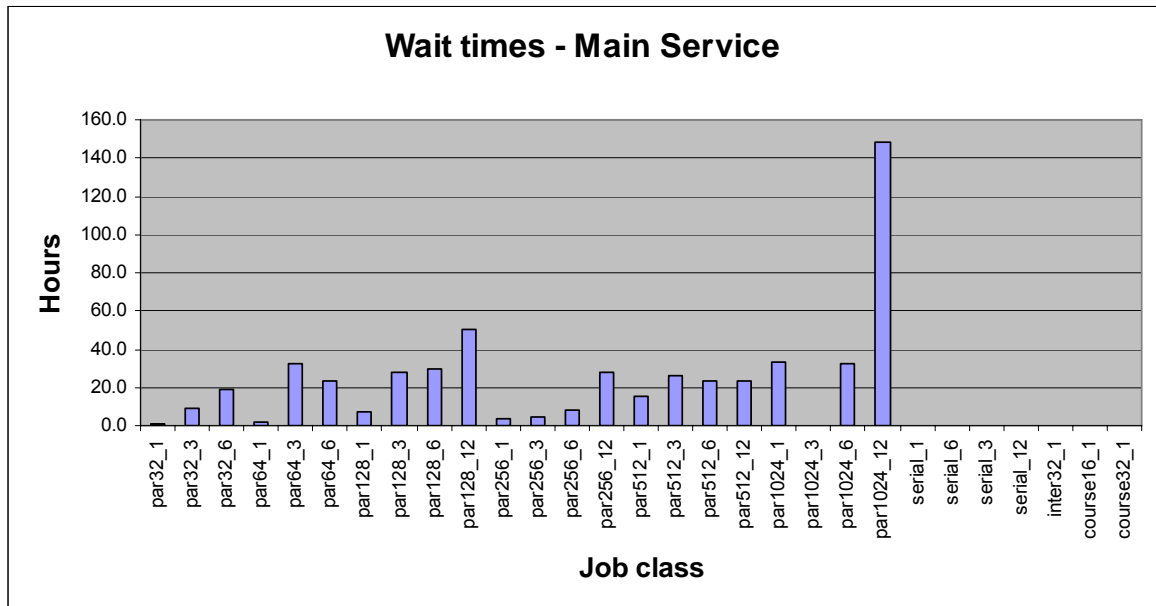


Job wait times

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. 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 18 jobs in this class included one such sequence of nine jobs and one of three, both from e42, and another sequence of two jobs, from e06.

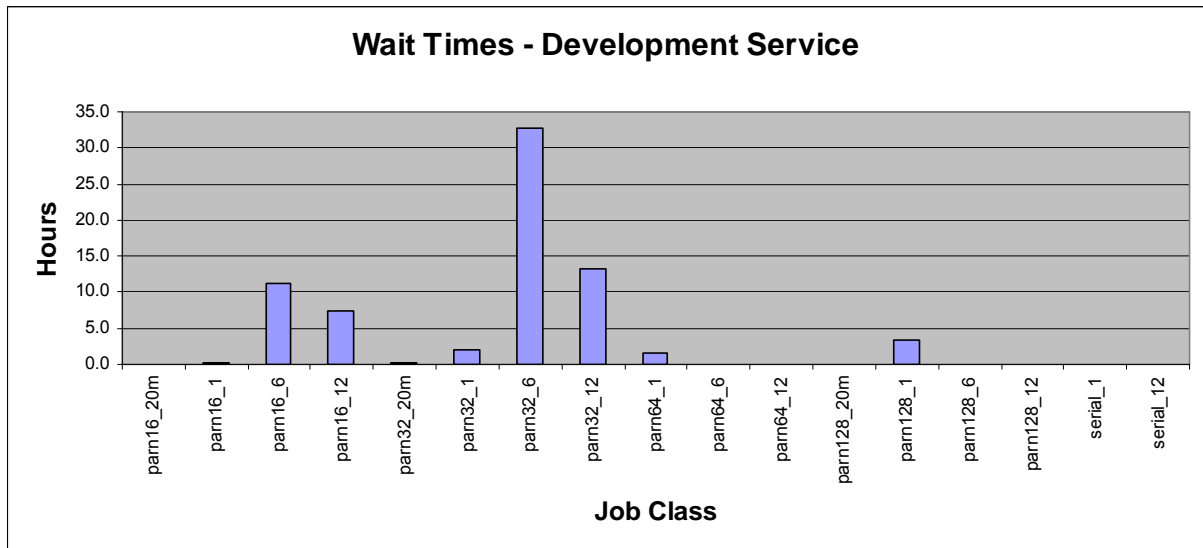
Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	Parallel	32	1	1.0	2255
par32_3	Parallel	32	3	9.2	281
par32_6	Parallel	32	6	18.5	715
par64_1	Parallel	64	1	1.8	712
par64_3	Parallel	64	3	32.2	35
par64_6	Parallel	64	6	23.2	226
par128_1	Parallel	128	1	7.0	203
par128_3	Parallel	128	3	28.0	44
par128_6	Parallel	128	6	29.6	70
par128_12	Parallel	128	12	50.7	93
par256_1	Parallel	256	1	3.5	216
par256_3	Parallel	256	3	4.9	36
par256_6	Parallel	256	6	8.0	71
par256_12	Parallel	256	12	27.5	111
par512_1	Parallel	512	1	15.6	49
par512_3	Parallel	512	3	26.4	4

par512_6	Parallel	512	6	23.8	5
par512_12	Parallel	512	12	22.9	53
par1024_1	Parallel	1024	1	33.2	34
par1024_3	Parallel	1024	3	0.0	0
par1024_6	Parallel	1024	6	32.0	2
par1024_12	Parallel	1024	12	148.3	18
serial_1	Serial	1	1	0.3	656
serial_6	Serial	1	6	0.3	85
serial_3	Serial	1	3	0.4	53
serial_12	Serial	1	12	0.2	93
inter32_1	interactive	32	1	0.0	3777
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.

<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	0.0	2049
parn16_1	Parallel	16	1 hour	0.1	1944
parn16_6	Parallel	16	6 hours	11.2	180
parn16_12	Parallel	16	12 hours	7.4	125
parn32_20m	Parallel	32	20 mins	0.3	392
parn32_1	Parallel	32	1 hour	1.9	786
parn32_6	Parallel	32	6 hours	32.8	317
parn32_12	Parallel	32	12 hours	13.1	202
parn64_1	Parallel	64	1 hour	1.5	558
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	3.3	33
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	6125
serial_12	Serial	1	12 hours	0.0	14



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

<i>Consortium</i>	<i>Usage (Tapes)</i>	<i>Quota (Tapes)</i>	<i>Files</i>	<i>Data (Gb)</i>
c01	2	2	7231	65
e01	43	43	147265	4112
e03	5	5	18797	429
e14	10	10	343257	582
e15	1	3	26	6
e24	7	10	6162	393
e26	2	2	545	27
e42	5	5	104	137
n01	213	220	28389	21698
n02	276	290	151080	33983
n04	28	30	116775	3740
z001	7	10	11045	67
z002	4	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	42	43.3
Technical	44	45.4
In-depth	11	11.3
PMR	0	0.0
TOTAL	97	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	91	93.8
Website	1	1.0
Other/general	5	5.2
TOTAL	97	100.0

Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	68	79.1	75%
Finished within 72 Hours	85	98.8	97%
Finished after 72 Hours	1	1.2	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	41	97.6	97%
Finished after 48 Hours	1	2.4	

Experts Handling Queries

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	34	18	9	0
dl.ac.uk	0	9	2	0
Sysadm	8	17	0	0
Other people	0	0	0	0

3.2 Training

No training courses were run this month.

4 Staffing

4.1 Science Support Staffing

Daresbury Laboratory

<i>Name</i>	<i>Days</i>
Ashworth	5.2
Blake	4.8
Bush	14.0
Guest	4.8
Johnstone	22.0
Jones	3.0
Plummer	5.5
Sherwood	2.6
Sunderland	22.0
Thomas	10.0
Pickles	2.2
Total (Days)	96.0
FTEs	5.4

EPCC

<i>Name</i>	<i>Days</i>
Simpson	18.1
Booth	18.4
Henty	7.3
Smith	12.6
Bull	3.2
Fisher	7.0
Hein	4.5
Jackson	3.9
Pringle	0.0
Reid	9.9
Stratford	7.3
Nazarova	4.0
Trew	4.3
Gray	10.1
D'Mellow	7.5
Hill	1.0

Johnson	0.6
Maynard	6.2
Other staff	42.0
Helpdesk	1.0
Total (Days)	168.6
FTEs	9.5

Overall Levels

	<i>FTEs</i>
DL	5.4
EPCC	9.5
Total	14.9

4.2 Systems Staffing

<i>Name</i>	<i>Days</i>
Andrews	10.4
Blake	0.0
Brown	22.0
Fisher	6.0
Georgeson	17.6
Franks	7.2
Jones	0.8
Shore	17.6
BITD	17.6
Total (days)	102.2
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%	99.9%
Technology MTBF (hours)	200	300	732
Number of AV FTEs	7.5	10	14.9
Number of training days per month	20/12	25/12	21/8
Non in-depth queries resolved within 3 days	85%	97%	98.8%
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 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