

# HPCx Service Report

## June 2006

### 1 Introduction

This report covers the period from 1 June 2006 at 0800 to 1 July 2006 at 0800, a service month of 720 hours.

Utilisation continued to recover, and has now passed 61%, although this is still below average. Utilisation of the capacity region, at 90%, is exceptionally high. There were no SEV1 incidents this month.

### 2 Usage

#### 2.1 Availability

##### *Incidents*

During this month, there were 14 incidents, none 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	0
2	0
3	13
4	1

The MTBF figures for this month were as follows:

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

## *Serviceability*

There was a total of 10.8 hours of scheduled downtime this month.

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

## 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	53565	115	258438	8.4%
e05	202169	252	954627	31.1%
e06	11981	446	59826	1.9%
e08	12593	0	60626	2.0%
e10	4410	0	21231	0.7%
e11	8965	0	43163	1.4%
e14	72067	131	347590	11.3%
e15	0	1	6	0.0%
e17	26996	0	129970	4.2%
e18	0	0	0	0.0%
e19	62	11	350	0.0%
e20	54	0	259	0.0%
e21	50	14	308	0.0%
e23	3	0	12	0.0%
e24	176	0	846	0.0%
e25	693	33	3497	0.1%
e26	739	0	3555	0.1%
e31	1476	15	7180	0.2%
e32	588	3	2842	0.1%
e33	7287	0	35084	1.1%
e35	94	120	1032	0.0%
e36	4677	0	22516	0.7%
e37	22517	2	108415	3.5%
e40	3960	0	19067	0.6%
e41	0	0	0	0.0%
e49	0	0	1	0.0%
e50	30	0	147	0.0%
<i>EPSRC Total</i>	435151	1141	2080588	67.8%

n01	72739	17	350280	11.4%
n02	34707	10	167144	5.4%
n03	10183	52	49277	1.6%
n04	27753	221	134679	4.4%
<i>NERC Total</i>	145382	301	701380	22.9%

p01	8742	0	42091	1.4%
<i>PPARC Total</i>	8742	0	42091	1.4%

c01	42125	21	202911	6.6%
<i>CCLRC Total</i>	42125	21	202911	6.6%

x01	2625	293	14048	0.5%
<i>External Total</i>	2625	293	14048	0.5%

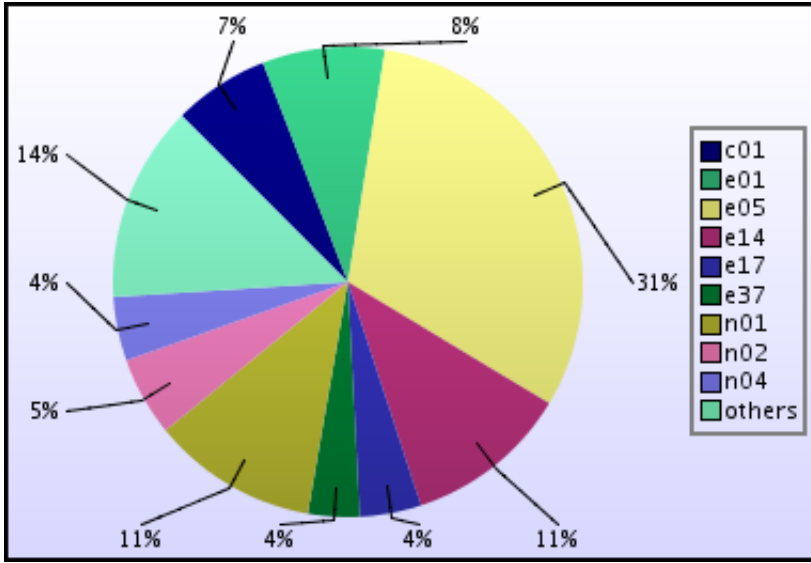
z001	5140	83	25142	0.8%
z002	5	0	26	0.0%
z004	565	24	2835	0.1%
<i>HPCx Total</i>	5710	107	28004	0.9%

c01	8927	3	42989	1.4%
<i>CCLRC Total</i>	8927	3	42989	1.4%

b08	9814	0	47250	1.6%
<i>BBSRC Total</i>	9814	0	47250	1.6%

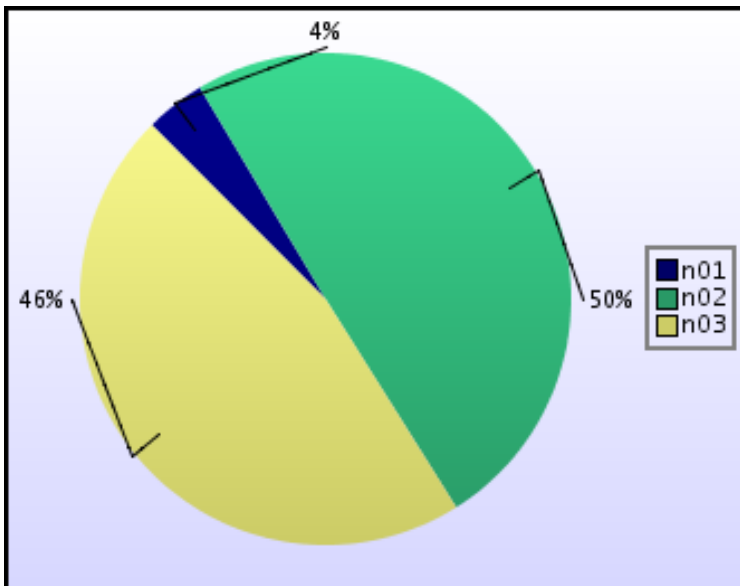
x01	1714	362	9996	0.3%
<i>External Total</i>	1714	362	9996	0.3%

z001	1858	11	8999	0.3%
z002	652	0	3138	0.1%
z004	3	0	15	0.0%
z05	350	0	1686	0.1%
z06	1	0	7	0.0%
<i>HPCx Total</i>	2864	12	13845	0.5%



*Development Service*

Consortium	CPU Hours (Parallel)	CPU Hours (Other)	AUs charged	%age of charged AUs
n01	3437	0	16546	3.9%
n02	43006	171	207872	49.6%
n03	40409	0	194547	46.4%
<i>NERC Total</i>	86852	171	418964	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	457394	14.9%	2720
33–64	287694	9.3%	738
65–128	549226	17.8%	249
129–256	937505	30.4%	363
257–512	703049	22.8%	116
513–1024	145101	4.7%	29

### *Utilisation by region*

*Capacity Region* (26 nodes, jobs using ≤128 CPUs): a total of 1294315 raw AUs were used; that is 89.8% of the total available in this region

*Capability Region* (64 nodes, jobs using >128 CPUs): a total of 1785656 raw AUs were used; that is 50.3% of the total available in this region

The remaining 2 nodes are reserved for interactive-parallel work.

Overall utilisation was 61.3%.

### *Development Service*

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	372710	89.1%	2713
33–64	28343	6.8%	121
65–128	17090	4.1%	76
129–256	0	0.0%	0

Overall utilisation was 63.8%.

## 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:

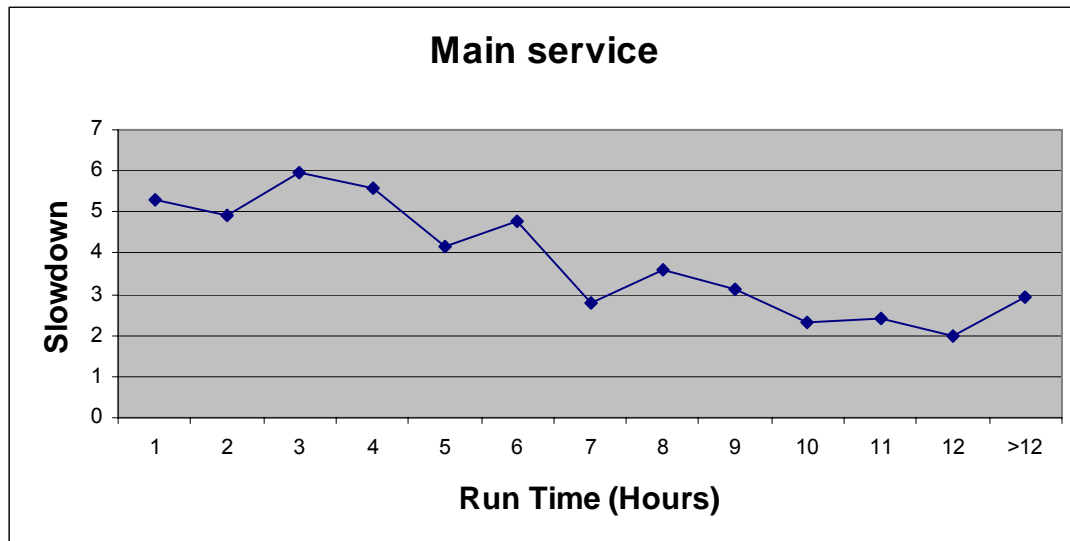
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

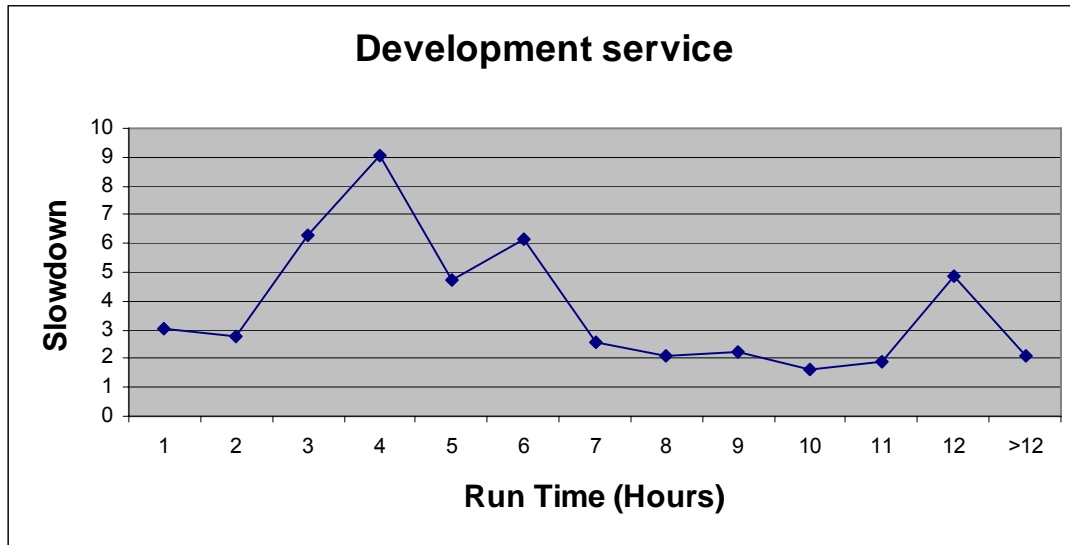
Slowdowns of less than around 10 are usually regarded as reasonable.

Despite the exceptional load on the capacity region, slowdowns on the main service are remarkably good. Slowdowns on the development service are also satisfactory.

### *Slowdowns by runtime*

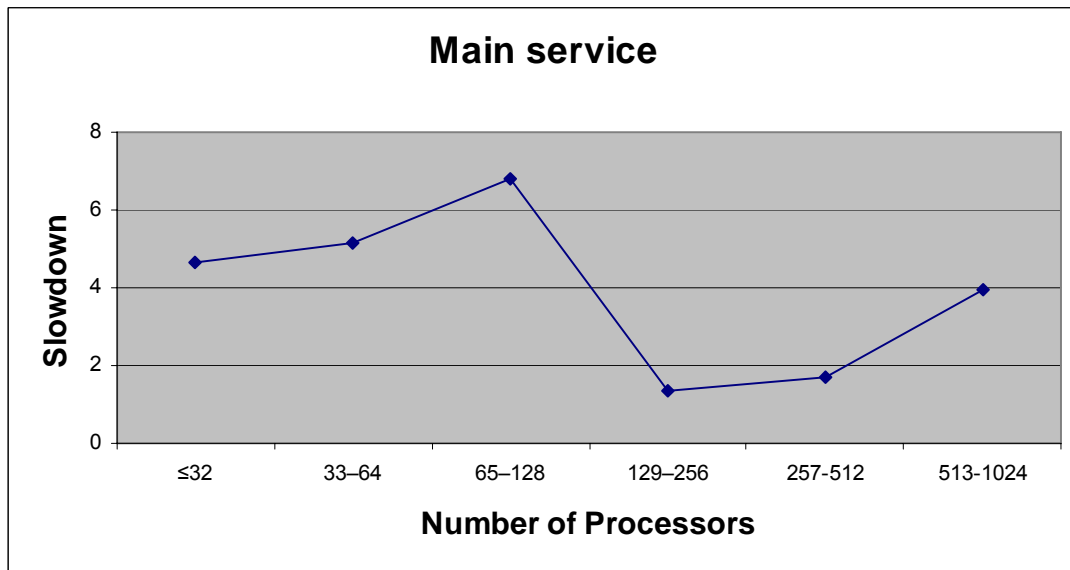
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

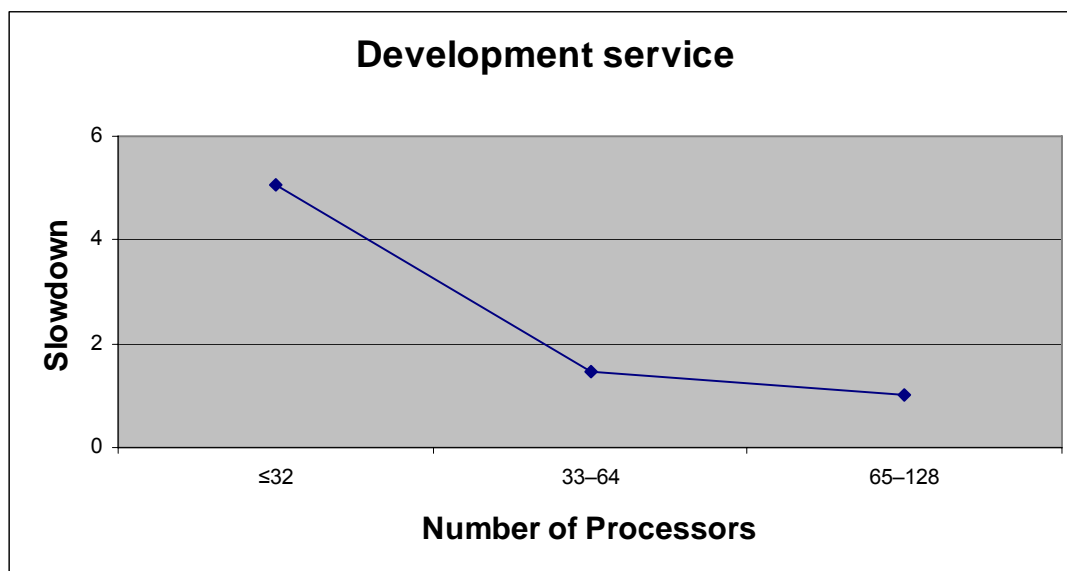




*Slowdowns by number of processors*

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..



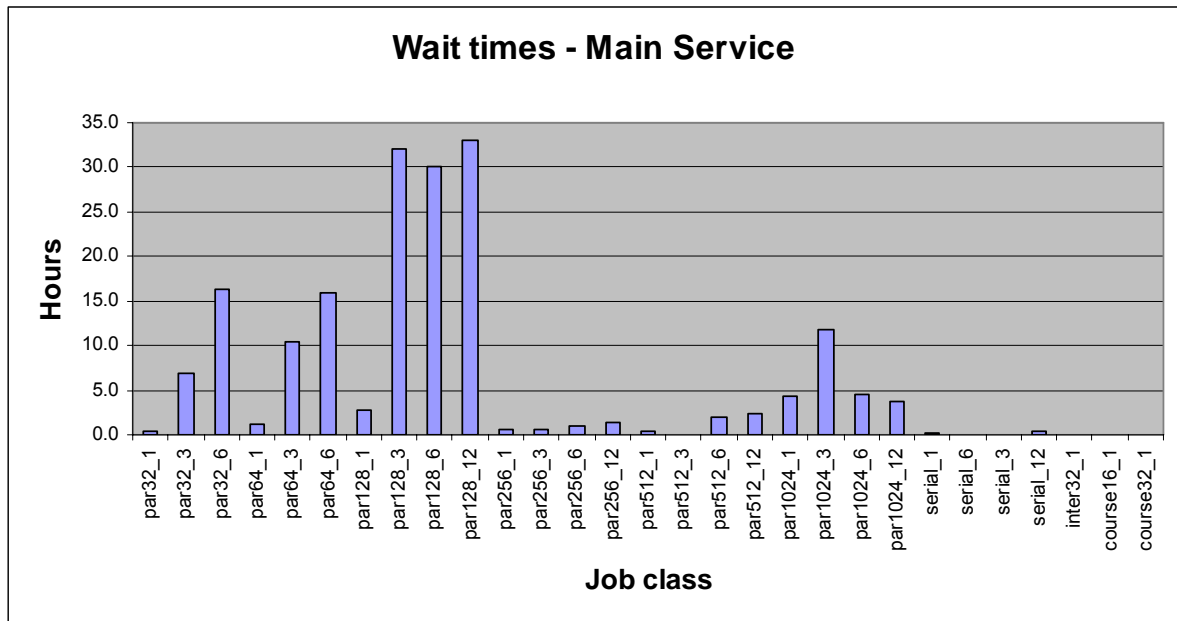


### Job wait times

The following table and graph shows the average wait time (in hours) for each class of job on the main service. The effects of the heavy utilisation of the capacity region can be clearly seen, but overall the figures are satisfactory.

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	parallel	32	1	0.4	1913
par32_3	parallel	32	3	6.8	151
par32_6	parallel	32	6	16.4	656
par64_1	parallel	64	1	1.1	483
par64_3	parallel	64	3	10.5	63
par64_6	parallel	64	6	16.0	192
par128_1	parallel	128	1	2.8	101
par128_3	parallel	128	3	32.1	3
par128_6	parallel	128	6	30.2	31
par128_12	parallel	128	12	33.0	114
par256_1	parallel	256	1	0.5	144
par256_3	parallel	256	3	0.6	59
par256_6	parallel	256	6	1.1	87
par256_12	parallel	256	12	1.5	73
par512_1	parallel	512	1	0.3	37
par512_3	parallel	512	3	0.0	2
par512_6	parallel	512	6	1.9	28
par512_12	parallel	512	12	2.3	49
par1024_1	parallel	1024	1	4.3	17
par1024_3	parallel	1024	3	11.8	5

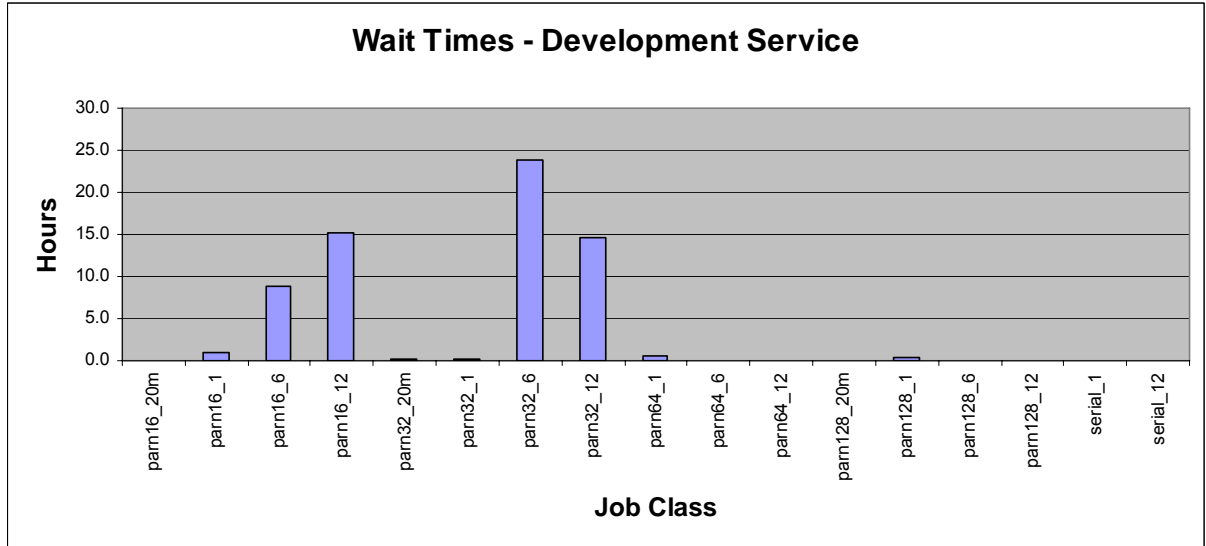
par1024_6	parallel	1024	6	4.5	1
par1024_12	parallel	1024	12	3.8	6
serial_1	serial	1	1	0.2	538
serial_6	serial	1	6	0.0	22
serial_3	serial	1	3	0.0	14
serial_12	serial	1	12	0.3	89
inter32_1	interactive	32	1	0.0	4151
course16_1	interactive	16	1	0.0	0
course32_1	parallel	32	1	0.0	0



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	137
parn16_1	parallel	16	1 hour	0.9	1664
parn16_6	parallel	16	6 hours	8.8	15
parn16_12	parallel	16	12 hours	15.2	78
parn32_20m	parallel	32	20 mins	0.2	180
parn32_1	parallel	32	1 hour	0.2	277
parn32_6	parallel	32	6 hours	23.9	158
parn32_12	parallel	32	12 hours	14.7	205
parn64_1	parallel	64	1 hour	0.7	121
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	0.5	76
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	2926
serial_12	serial	1	12 hours	0.0	0



## 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	34058.1	50,000
b03	52710.5	50,000
b08	703.9	50,000
c01	110684.1	150,000
e01	39958.6	48,829
e02	23079.3	38,829
e03	55181.2	225,012
e05	238267.6	450,500
e06	259961.5	300,000
e07	12890.9	20,000
e08	40804.7	50,000
e10	27490.4	150,000
e11	36980.8	100,000
e14	63537.1	100,000
e15	31529.8	50,000
e16	132.9	20,000
e17	19496.2	50,000
e18	26953.0	40,000
e19	1315.1	40,000
e20	56313.9	60,000
e21	354.4	50,000
e22	127.9	10,000
e23	57.8	50,000
e24	48250.6	200,000
e25	8177.7	50,000
e26	13940.2	20,000
e27	7042.5	20,000
e29	2127.1	30,000
e30	0.1	40,000
e31	40245.7	50,000
e32	46942.5	50,000
e33	131.1	50,000
e34	0.1	50,000
e35	2803.4	100,000
e36	18860.0	50,000
e37	76331.8	100,000
e39	0.1	50,000
e40	4676.1	50,000

e41	1640.2	100,000
e42	7.1	50,000
e45	0.1	50,000
e46	0.1	50,000
e47	0.1	50,000
e48	4.8	50,000
e49	75.6	50,000
e50	338.2	10,000
e51	0.1	50,000
e52	0.4	50,000
e53	794.7	50,000
e54	12.2	50,000
e55	0.3	50,000
n01	45638.2	100,000
n02	100715.2	128,000
n03	65833.9	100,000
n04	229233.8	299,999
p01	107824.3	200,000
x01	44632.7	50,000
x02	8746.2	20,000
x03	634.6	50,000
z001	250084.0	270,001
z002	31895.6	48,001
z003	0.2	3
z004	97381.3	100,000
z05	4188.4	30,000
z06	48034.3	50,000
z07	27032.6	50,000
z09	15366.4	50,000

### Workspace

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
b02	14.8	1,025
b03	47907.9	100,000
b08	5019.5	50,000
c01	86105.8	100,000
e01	714671.1	1,249,995
e02	8354.8	10,000
e03	9.8	500,000
e05	212836.4	498,004
e06	285588.8	400,000
e07	81641.6	99,999
e08	140.8	5,000
e10	284222.9	400,000
e11	22561.8	100,000

e14	104486.2	150,000
e15	31540.2	100,000
e16	0.2	60,000
e17	2014.0	100,000
e18	18431.3	80,000
e19	169044.5	200,000
e20	926743.0	1,000,000
e21	1.1	100,000
e22	0.1	20,000
e23	0.1	100,000
e24	73813.8	500,000
e25	136301.3	150,000
e26	0.1	40,000
e27	0.3	40,000
e29	5296.1	8,000
e30	0.1	80,000
e31	96128.1	100,000
e32	90365.8	100,000
e33	389.1	100,000
e34	0.1	100,000
e35	0.2	200,000
e36	0.1	50,000
e37	21765.4	150,000
e39	0.1	100,000
e40	0.2	100,000
e41	0.2	200,000
e42	1.5	100,000
e45	0.1	100,000
e46	0.1	50,000
e47	0.1	160,000
e48	0.1	200,000
e49	0.2	50,000
e50	0.3	100,000
e51	0.1	100,000
e52	0.1	50,000
e53	0.2	150,000
e54	0.2	100,000
e55	0.1	100,000
n01	288903.3	800,000
n02	1819303.0	2,049,003
n03	21.5	41,002
n04	746812.6	750,000
p01	41764.4	50,000
x01	95937.3	160,000
x02	0.2	20,000
x03	177.6	50,000
z001	397423.7	399,999
z002	388.3	770

z003	0.2	3
z004	23740.0	25,000
z05	4739.7	20,000
z06	71343.8	100,000
z07	8.3	20,000
z09	53680.4	100,000

*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	500,000
n02	3,121,136	5,210,003
n04	0	100,001

## 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	7229	52
e01	42	43	117452	3824
e03	5	5	18797	429
e14	9	10	165658	309
e15	1	3	26	6
e26	2	2	545	27
n01	182	220	22390	18979
n02	216	290	117300	26821
n04	30	30	110306	3255
z001	2	10	6189	50
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	48	40.0
Technical	62	51.7
In-depth	8	6.7
PMR	2	1.7
TOTAL	120	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	113	94.2
Website	4	3.3
Other/general	3	2.5
TOTAL	120	100.0

##### *Performance*

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	95	86.4	75%
Finished within 72 Hours	109	99.1	97%
Finished after 72 Hours	1	0.9	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	48	100.0	97%
Finished after 48 Hours	0	0.0	

##### *Experts Handling Queries*

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	31	24	1	0
dl.ac.uk	3	15	4	2
Sysadm	13	23	3	0
Other people	1	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	12.7
Blake	2.0
Bush	22.0
Guest	5.3
Johnstone	11.0
Jones	4.4
Plummer	7.5
Sherwood	0.0
Sunderland	19.0
Thomas	0.0
Pickles	1.8
van Dam	0.0
Total (Days)	85.6
FTEs	4.8

#### *EPCC*

<i>Name</i>	<i>Days</i>
Simpson	18.1
Booth	13.5
Henty	11.8
Smith	12.5
Bull	11.5
Fisher	6.0
Hein	11.8
Jackson	2.5
Pringle	0.9
Reid	6.3
Stratford	10.2
Nazarova	8.2
Trew	4.3
Gray	7.9
D'Mellow	12.9
Hill	0.9

Johnson	0.3
Beckett	0.4
Other staff	20.0
Helpdesk	0.0
Training	1.7
<b>Total (Days)</b>	<b>161.7</b>
<b>FTEs</b>	<b>9.1</b>

*Overall Levels*

	<i>FTEs</i>
DL	4.8
EPCC	9.1
<b>Total</b>	<b>13.9</b>

**4.2 Systems Staffing**

<i>Name</i>	<i>Days</i>
Andrews	16.5
Blake	0.0
Brown	22.0
Fisher	12.5
Georgeson	12.8
Franks	15.8
Jones	1.1
Shore	5.3
BITD	17.6
<b>Total (days)</b>	<b>103.5</b>
<b>FTEs</b>	<b>5.8</b>

*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	13.9
Number of training days per month	20/12	25/12	21/6
Non in-depth queries resolved within 3 days	85%	97%	99.1%
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

<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 Decananometer 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
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
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
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
x02		OHM Ltd	Dr Lucy MacGregor
n05	2	Non-linear Wave-particle Instabilities in Plasmas	Dr Mervyn Freeman