

# HPCx Service Report

## June 2007

### 1 Introduction

This report covers the period from 0800 on 1 June 2007 to 0800 on 1 July 2007, a service month of 720 hours.

After last month's drop, utilisation returned to a very high level at nearly 81%. Utilisation of the development service continues to be exceptionally high, at more than 94%. For the fifth month running, there were no SEV1 incidents;

### 2 Usage

#### 2.1 Availability

##### *Incidents*

During this month, there was one incident, which was not at SEV1. The following table indicates the severity levels of the incidents, where SEV1 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	1
4	0

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*

Scheduled downtime for this month was 8.8 hours.

<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	169505	388	768053	11.9%
e05	214694	449	1022654	15.8%
e06	4113	8	19841	0.3%
e08	29190	1	140535	2.2%
e10	7782	15	37538	0.6%
e11	45959	0	221266	3.4%
e17	76	0	368	0.0%
e18	979	1	4717	0.1%
e24	333614	5	1606188	24.8%
e26	442	0	2130	0.0%
e31	5812	18	28069	0.4%
e33	22035	12	106141	1.6%
e35	81369	92	392192	6.1%
e36	10876	0	45069	0.7%
e37	75682	0	364371	5.6%
e38	18	0	85	0.0%
e39	18642	5	89774	1.4%
e41	530	0	2552	0.0%
e42	78239	0	376678	5.8%
e46	282	0	1357	0.0%
e49	475	1	2292	0.0%
e50	2527	0	12164	0.2%
e53	308	60	1772	0.0%
e59	0	10	51	0.0%
e60	23370	0	112513	1.7%
e61	18200	14	87694	1.4%
<i>EPSRC Total</i>	1144717	1080	5446063	84.1%

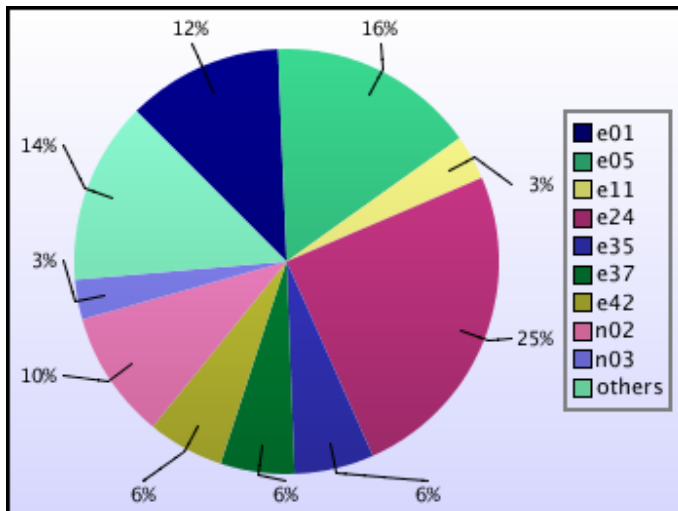
n01	22657	0	109080	1.7%
n02	131477	15	633063	9.8%
n03	43076	52	195939	3.0%
n04	5567	66	27123	0.4%
<i>NERC Total</i>	202777	133	965203	14.9%

p01	2836	17	13738	0.2%
<i>PPARC Total</i>	2836	17	13738	0.2%

c01	986	5	4771	0.1%
<i>CCLRC Total</i>	986	5	4771	0.1%

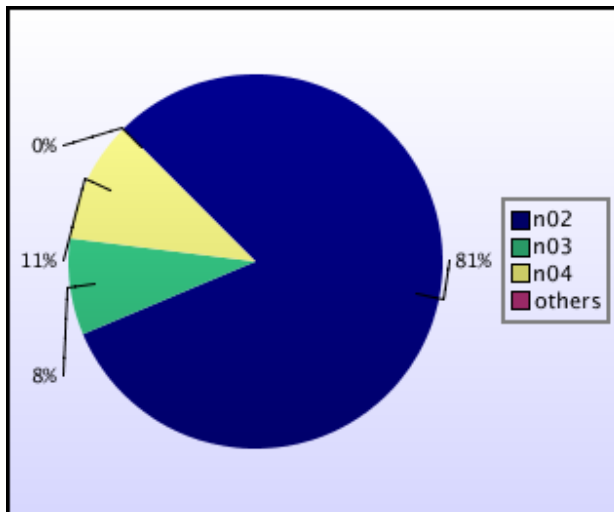
x01	8310	2	40021	0.6%
<i>External Total</i>	8310	2	40021	0.6%

z001	701	1	3379	0.1%
z004	1082	20	5305	0.1%
z06	37	0	176	0.0%
<i>HPCx Total</i>	1820	21	8862	0.1%



### Development Service

Consortium	CPU Hours (Parallel)	CPU Hours (Other)	AUs charged	%age of charged AUs
n01	0	0	0	0.0%
n02	104323	198	503207	81.2%
n03	10701	0	51520	8.3%
n04	13557	0	65269	10.5%
<i>NERC Total</i>	128581	198	619996	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	532487	8.1%	3188
33–64	363715	5.5%	1410
65–128	1648331	25.1%	2135
129–256	2624954	40.0%	546
257–512	1294322	19.7%	181
513–1024	90808	1.4%	21

Overall utilisation of the main service was 80.8%. Capability usage was 21.1% of the total.

#### *Development Service*

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	553471	89.4%	6406
33–64	65573	10.6%	351

Overall utilisation of the development service was 94.2%.

## 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:

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

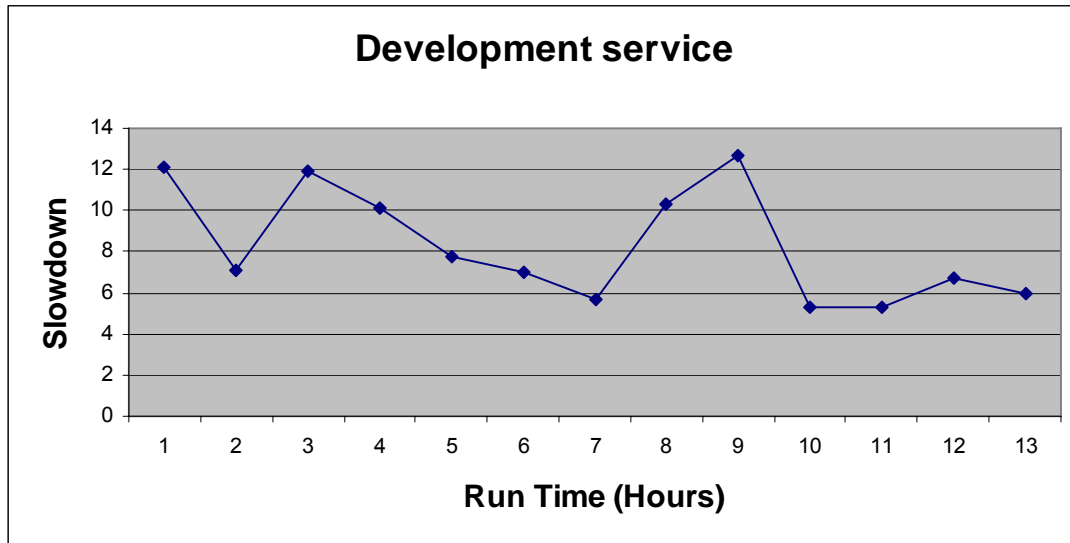
Slowdowns of less than around 10 are usually regarded as reasonable.

On both services, slowdowns are currently generally satisfactory, except as noted below.

### *Slowdowns by runtime*

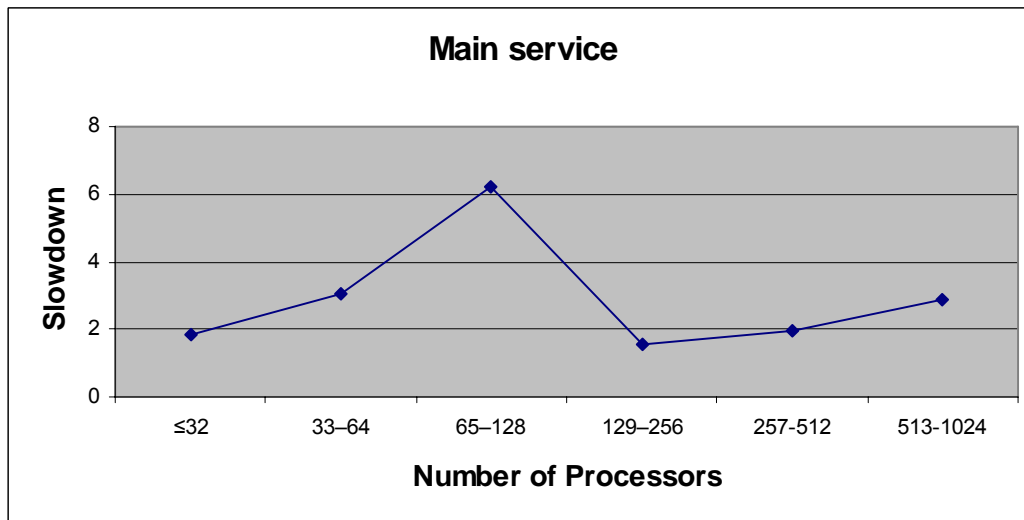
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.



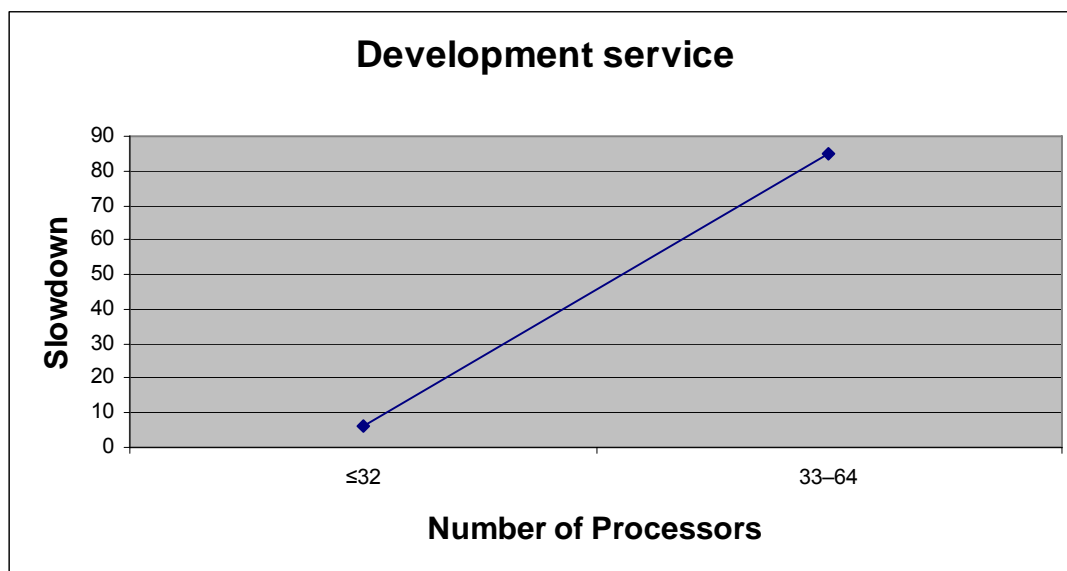


*Slowdowns by number of processors*

In the graphs below, we plot the slowdown figures against the number of processors used. Only jobs which ran for more than 1 hour are included.



Figures on the development service (see below) were distorted by the actions of a single user who submitted jobs and then deliberately held them, in an attempt to manipulate the queuing system to his advantage. The user was asked to stop this behaviour, which he has now done.

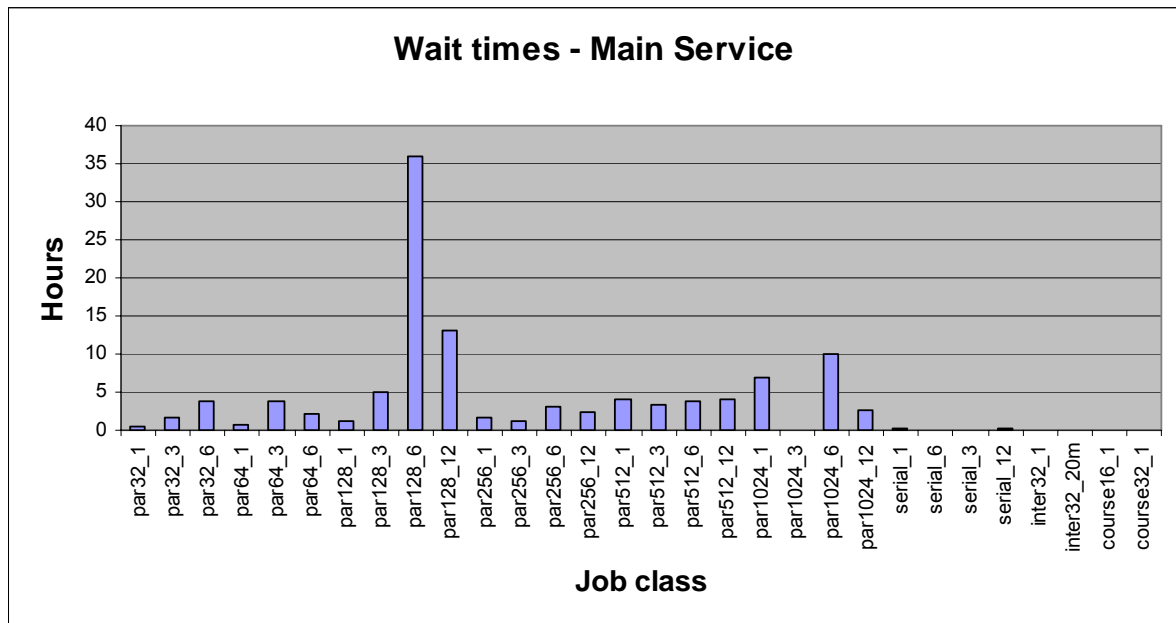


#### Job wait times – main service

The following table and graph shows the average wait time (in hours) for each class of job on the main service. Once again, the long wait times for long 128-processor jobs are attributable to the high utilisation of the capacity region.

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	parallel	32	1	0.4	2308
par32_3	parallel	32	3	1.7	70
par32_6	parallel	32	6	3.9	810
par64_1	parallel	64	1	0.7	404
par64_3	parallel	64	3	3.8	52
par64_6	parallel	64	6	2.0	954
par128_1	parallel	128	1	1.2	1732
par128_3	parallel	128	3	5.0	80
par128_6	parallel	128	6	35.9	176
par128_12	parallel	128	12	13.1	147
par256_1	parallel	256	1	1.7	88
par256_3	parallel	256	3	1.1	93
par256_6	parallel	256	6	3.1	73
par256_12	parallel	256	12	2.5	292
par512_1	parallel	512	1	4.0	76
par512_3	parallel	512	3	3.3	20
par512_6	parallel	512	6	3.8	16
par512_12	parallel	512	12	4.0	69
par1024_1	parallel	1024	1	6.8	17
par1024_3	parallel	1024	3	0.0	0

par1024_6	parallel	1024	6	10.1	2
par1024_12	parallel	1024	12	2.6	2
serial_1	serial	1	1	0.3	4596
serial_6	serial	1	6	0.0	34
serial_3	serial	1	3	0.0	19
serial_12	serial	1	12	0.3	88
inter32_1	interactive	32	1	0.0	961
inter32_20m	interactive	32	1	0.0	2346
course16_1	interactive	16	1	0.0	0
course32_1	parallel	32	1	0.0	0

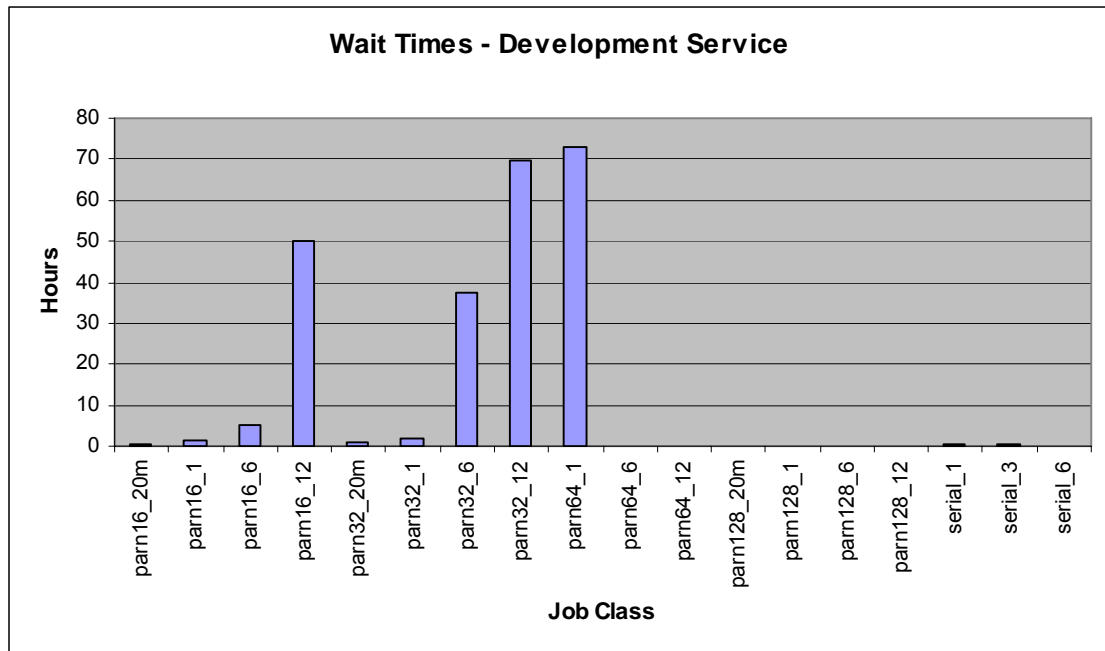


*Job wait times – development service*

As we noted last month, wait times on the development service have lengthened to some degree, as a result of the exceptionally high utilisation of the service (94.2%). For the one-hour 64-processor jobs, see the note regarding slowdowns above.

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
parn16_20m	parallel	16	20 mins	0.3	809
parn16_1	parallel	16	1 hour	1.4	3192
parn16_6	parallel	16	6 hours	5.3	502
parn16_12	parallel	16	12 hours	49.9	111
parn32_20m	parallel	32	20 mins	1.1	354
parn32_1	parallel	32	1 hour	1.9	1238

parn32_6	parallel	32	6 hours	37.5	96
parn32_12	parallel	32	12 hours	69.8	104
parn64_1	parallel	64	1 hour	73.2	351
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	0.0	0
parn128_6	parallel	128	6 hours	0.0	0
parn128_12	parallel	128	12 hours	0.0	0
serial_1	serial	1	1 hour	0.3	3502
serial_3	serial	1	12 hours	0.5	22
serial_6	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	50,000
b03	52,711	50,000
b08	18,652	50,000
c01	149,366	300,000
e01	183,496	199,995
e03	59,162	225,012
e05	344,740	614,550
e06	286,462	300,000
e08	99,253	100,000
e10	97,235	150,000
e11	43,038	100,000
e14	93,165	100,000
e15	40,730	50,000
e16	133	20,000
e17	48,574	50,000
e18	36,462	40,000
e19	1,417	40,000
e20	57,803	60,000
e21	1,521	50,000
e22	5,268	10,000
e23	9,733	50,000
e24	62,545	394,376
e25	24,470	50,000
e26	18,060	20,000
e27	19,054	20,000
e29	23,455	50,000
e30	0	40,000
e31	31,090	50,000
e32	47,110	50,000
e33	14,001	50,000
e34	0	50,000
e35	74,514	100,000
e36	49,084	100,000
e37	125,694	204,800
e38	15,042	50,000
e39	39,667	150,000
e40	18,109	50,000
e41	1,532	100,000

e42	34,124	100,000
e44	56	50,000
e45	43,936	50,000
e46	6,654	50,000
e47	0	50,000
e48	5	50,000
e49	33,981	50,000
e50	3,257	13,000
e51	4,469	50,000
e52	11	50,000
e53	2,876	50,000
e54	46,526	50,000
e55	1,664	50,000
e56	47,509	50,000
e57	0	50,000
e58	19,291	100,000
e59	257	100,000
e60	46,728	50,000
e61	18,992	50,000
n01	107,707	250,000
n02	165,065	298,000
n03	71,791	100,000
n04	286,015	299,999
p01	164,687	200,000
x01	48,484	50,000
x02	8,746	20,000
x03	4,227	50,000
z001	478,886	500,000
z002	45,347	124,000
z003	0	3
z004	93,849	100,000
z05	4,188	30,000
z06	59,512	75,000
z07	35,518	50,000
z10	983	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	5,100	50,000
c01	89,093	100,000
e01	1,229,996	1,249,995
e03	10	500,000
e05	425,977	662,006

e06	367,941	400,000
e08	141	5,000
e10	342,086	400,000
e11	46,482	100,000
e14	196,315	250,000
e15	36,691	100,000
e16	0	60,000
e17	97,381	100,000
e18	35,732	80,000
e19	169,244	200,000
e20	941,925	1,000,000
e21	1	100,000
e22	0	20,000
e23	37,389	100,000
e24	1	2,800,000
e25	139,279	150,000
e26	0	40,000
e27	2,760	40,000
e29	7	9,800
e30	0	80,000
e31	84,028	100,000
e32	99,998	100,000
e33	55,574	100,000
e34	0	100,000
e35	8,469	200,000
e36	49,449	200,000
e37	221,634	307,200
e38	0	100,000
e39	0	100,000
e40	1	100,000
e41	142,251	200,000
e42	253,047	400,000
e44	0	100,000
e45	0	100,000
e46	0	50,000
e47	0	160,000
e48	95,722	200,000
e49	25,224	50,000
e50	217,620	100,000
e51	0	100,000
e52	0	50,000
e53	771	150,000
e54	0	100,000
e55	0	100,000
e56	99,999	100,000
e57	0	100,000
e58	0	200,000
e59	0	100,000

e60	0	100,000
e61	24,456	100,000
n01	330,426	800,000
n02	6,835,834	8,499,904
n03	24,614	81,002
n04	519,079	750,000
p01	41,764	50,000
x01	159,995	160,000
x02	0	20,000
x03	178	50,000
z001	462,210	500,000
z002	1,617	770
z003	0	3
z004	21,560	25,000
z05	4,740	20,000
z06	57,096	100,000
z07	4	20,000
z10	0	50,000

*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>
n02	5,943,533	9,499,003
n04	315,159	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	7,231	65
e01	60	70	291,961	5,833
e03	5	5	18,797	429
e14	10	10	391,623	595
e15	1	3	26	6
e24	10	10	7,785	803
e26	2	2	545	27
e42	10	10	29,481	447
n01	302	305	34,273	32,399
n02	524	555	610,385	57,060
n04	28	30	116,775	3,740
z001	7	10	11,045	67
z002	3	4	5,802	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

The format of this section has evolved this month, reflecting the advent of the new SAFE-based helpdesk software.

##### *Classifications*

<i>Service metric</i>	<i>Number</i>	<i>% of all</i>
Administrative	27	44.3%
Technical	25	41.0%
In-depth	7	11.5%
Technical assessment	2	3.3%
PMR	0	0.0%
<i>Total</i>	61	100.0%

The *PMR* service metric includes in-depth queries that result in Problem Management Reports for IBM. The *Technical Assessment* metric has been added since technical assessments are now being handled through the helpdesk, for compatibility with the HECToR procedure.

In place of the former *Service Area* information we shall supply a breakdown of queries by subject category.

<i>Category</i>	<i>Number</i>	<i>% of all</i>
Disks, tapes, resources	17	27.9%
3rd party software	10	16.4%
Login, passwords, ssh	9	14.8%
Access to HPCx	8	13.1%
None	5	8.2%
SAFE	4	6.6%
Batch system and queues	3	4.9%
Compilers and system software	2	3.3%
User behaviour	1	1.6%
Tools	1	1.6%
Porting	1	1.6%
<i>Total</i>	61	100.0%

*Performance*

<i>Metric</i>	<i>Achieved</i>	<i>Total</i>	<i>Fraction</i>	<i>Target</i>
Administrative queries - two days	25	27	93%	97%
All queries - three days	46	52	88%	97%
All queries - one day	37	52	71%	75%

*Query handlers*

<i>Handler</i>	<i>Technical</i>	<i>In-depth</i>	<i>Admin</i>	<i>PMR</i>	<i>Technical assessment</i>
Sysadm	16	2	10	0	
DL	6	2	1	1	
EPCC	20	8	17	0	

## **3.2 Training**

There were no training courses this month.

## 4 Staffing

### 4.1 Science Support Staffing

#### *Daresbury Laboratory*

<i>Name</i>	<i>Days</i>
Ashworth	15.4
Blake	0.0
Bush	21.0
Johnstone	0.0
Jones	2.0
Plummer	10.5
Sunderland	21.0
Todorov	10.5
<i>Total (Days)</i>	80.4
<i>FTEs</i>	4.5

#### *EPCC*

<i>Name</i>	<i>Days</i>
Simpson	12.2
Booth	13.6
Henty	7.9
Smith	0.0
Bull	8.8
Fisher	1.8
Hein	17.2
Jackson	1.6
Reid	21.2
Stratford	1.6
Nazarova	5.5
Trew	4.3
Gray	9.1
D'Mellow	16.2
Hill	9.5
Johnson	0.2

Maynard	0.7
Weiland	19.0
Piotrowski	5.7
Collard	0.8
<i>Total (Days)</i>	156.5
<i>FTEs</i>	8.8

*Overall Levels*

	<i>FTEs</i>
DL	4.5
EPCC	8.8
<i>Total</i>	13.3

**4.2 Systems Staffing**

<i>Name</i>	<i>Days</i>
Andrews	13.6
Brown	20.0
Fisher	10.7
Georgeson	18.9
Franks	17.1
Jones	1.0
BITD	21.0
<i>Total (days)</i>	102.3
<i>FTEs</i>	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%	100.0%
Technology MTBF (hours)	200	300	∞
Number of AV FTEs	7.5	10	13.3
Number of training days per month	20/12	25/12	13/6
Non in-depth queries resolved within 3 days	85%	97%	88.5%
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
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
e44	1	Extreme Wave Loading on Offshore Wave Energy Devices	Dr Deborah Greaves
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
e57	1	Triplex DNA Structures	Dr Hooshang Nikjoo
e58	1	Quantum Simulations for Chemical Biology	Dr Carmen Domene
e59	1	Turbulence in breaking gravity waves	Prof Ian Castro
e60	1	Device Electronics Based on nanoWires and NanoTubes	Dr Merlyne M de Souza
e61	1	Enhancement of droplet concentrations in clouds	Dr Alan A M Gadian

### 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
z10	Globus	Dr Stephen P Booth

## 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
e07	2	Turbulent Plasma Transport in Tokamaks	Dr Colin M Roach