

HPCx Service Report

September 2007

1 Introduction

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

Overall utilisation of the main service was just under 57%. Utilisation of the development service continues to be high, at nearly 88%.

2 Usage

2.1 Availability

Incidents

There were no SEV1 incidents again this month. The scheduled down time was only 5 hours 45 minutes, for the maintenance session on 12/9/2007.

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

<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	314788	257	1507157	33.2%
e05	215819	649	1035496	22.8%
e08	11732	0	56485	1.2%
e17	329	0	1584	0.0%
e18	838	0	4035	0.1%
e19	300	0	1442	0.0%
e24	57	2	284	0.0%
e33	67048	16	322875	7.1%
e35	69002	418	334222	7.4%
e36	4295	0	17574	0.4%
e39	19831	0	95476	2.1%
e41	1549	0	7456	0.2%
e42	34753	67	167639	3.7%
e44	0	0	1	0.0%
e45	15392	0	74103	1.6%
e49	11052	98	53680	1.2%
e50	8354	0	40218	0.9%
e53	2893	458	16134	0.4%
e59	1533	0	7381	0.2%
e60	15782	0	75983	1.7%
e61	3803	25	18429	0.4%
<i>EPSRC Total</i>	<i>803932</i>	<i>1992</i>	<i>3860686</i>	<i>85.1%</i>

n01	2812	0	13536	0.3%
n02	35576	6	171308	3.8%
n03	38502	287	159311	3.5%
n04	56619	46	251487	5.5%
<i>NERC Total</i>	<i>133509</i>	<i>338</i>	<i>595642</i>	<i>13.1%</i>

p01	2376	2	11446	0.3%
<i>PPARC Total</i>	<i>2376</i>	<i>2</i>	<i>11446</i>	<i>0.3%</i>

c01	2763	5	13326	0.3%
<i>CCLRC Total</i>	<i>2763</i>	<i>5</i>	<i>13326</i>	<i>0.3%</i>

b08	1176	0	5661	0.1%
<i>BBSRC Total</i>	1176	0	5661	0.1%

x01	839	0	4037	0.1%
<i>External Total</i>	839	0	4037	0.1%

z001	9151	2	44066	1.0%
z004	335	1	1614	0.0%
<i>HPCx Total</i>	9486	3	45681	1.0%

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>
n02	116206	121	560052	97.0%
n03	1688	16	8204	1.4%
n04	1902	7	9190	1.6%
<i>NERC Total</i>	119796	144	577446	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	431223	9.4%	3201
33–64	261592	5.7%	491
65–128	1160500	25.3%	680
129–256	1589118	34.6%	603
257–512	904428	19.7%	311
513–1024	246470	5.4%	28
>1024	38	0.0%	1

Overall utilisation of the main service was nearly 57%. Capability usage was 25% of the total.

Development Service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	561405	97.3%	5431
33–64	13174	2.3%	94
65–128	1479	0.3%	7
129–256	694	0.1%	1

Overall utilisation of the development service was nearly 88%.

2.4 Slowdown and Job Wait Times

Slowdowns

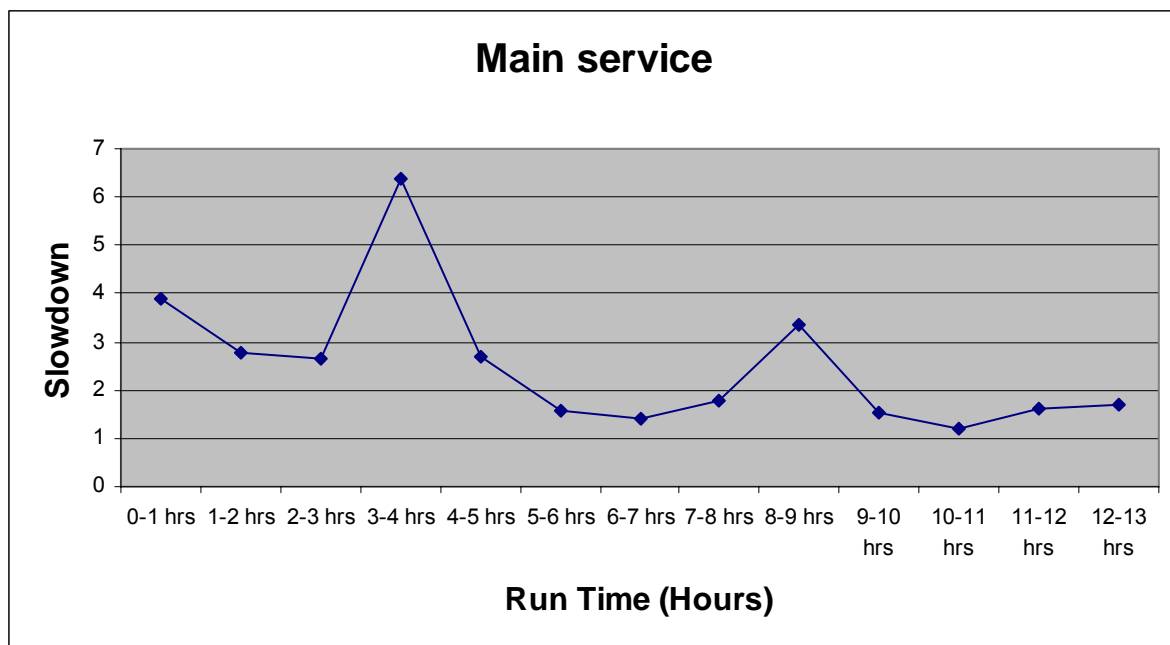
Slowdown is a widely used measure of the relative wait times of different classes of jobs. It is defined as:

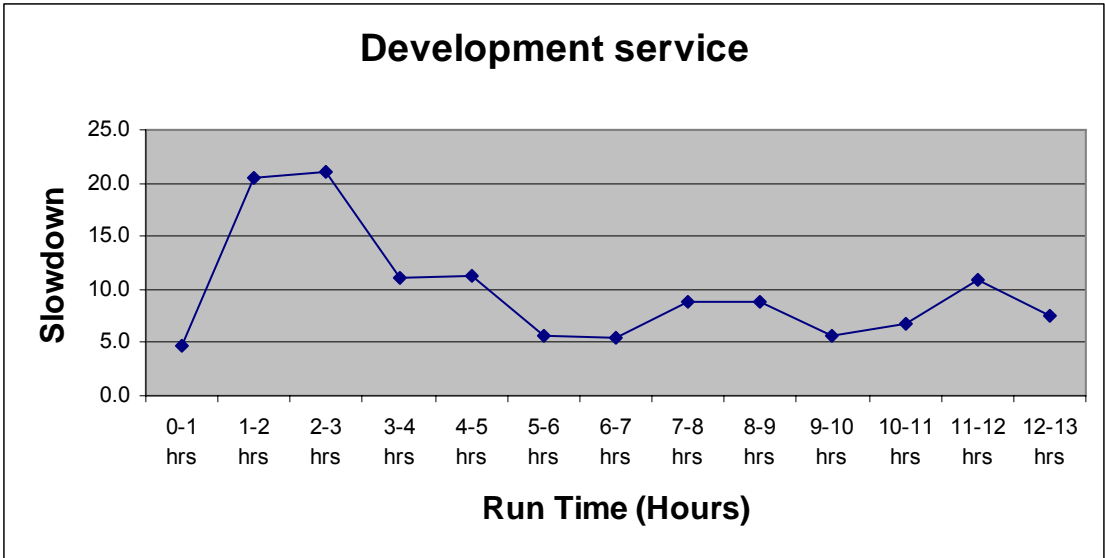
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

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

Slowdowns by runtime

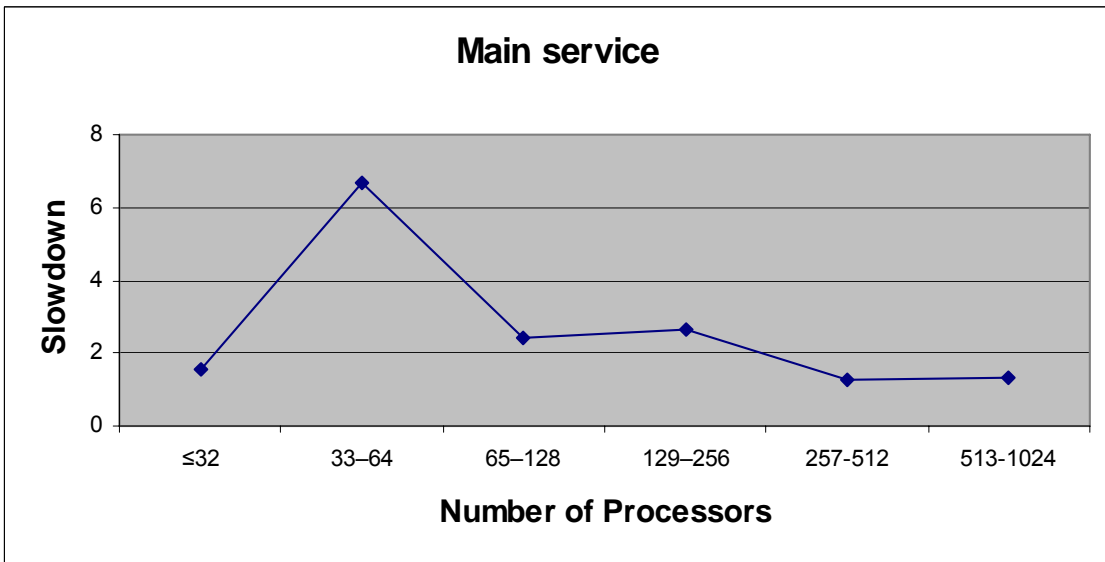
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

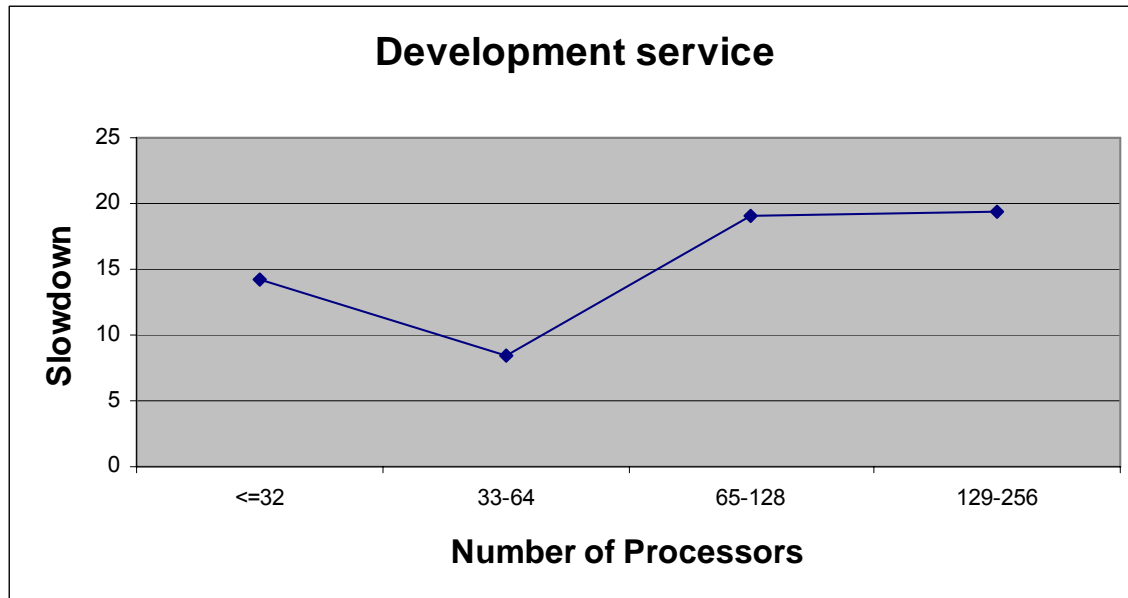




Slowdowns by number of processors

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.



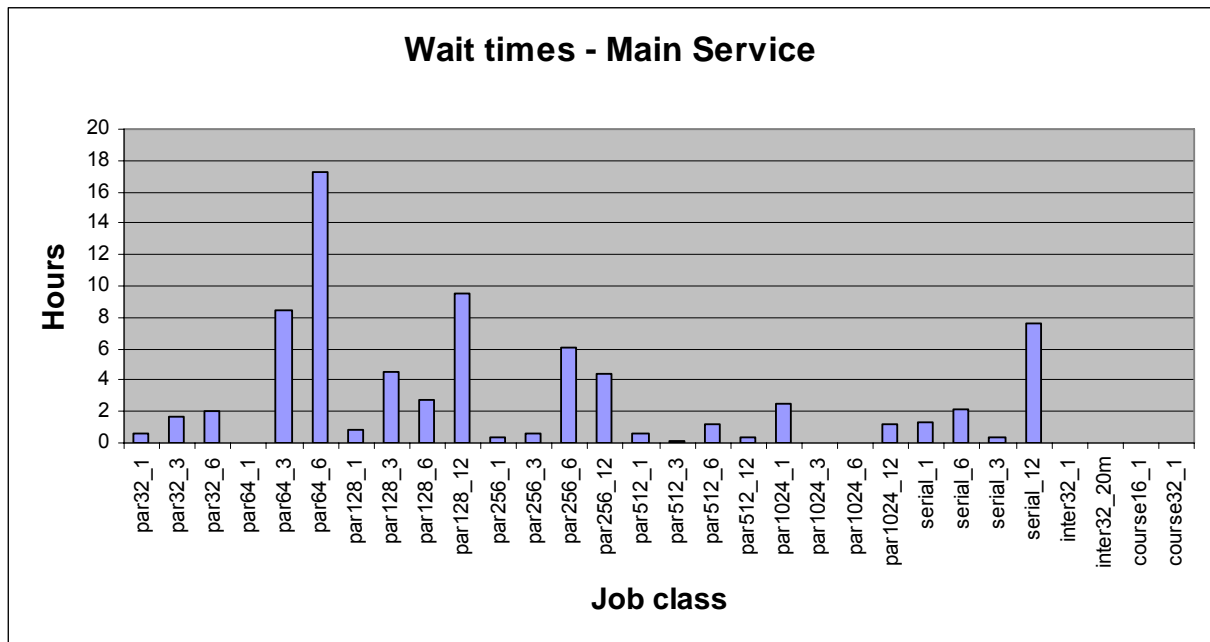


Job wait times – main service

The following table and graph shows the average wait time (in hours) for each class of job on the main service.

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
par32_1	parallel	32	1 hour	0.5	2169
par32_3	parallel	32	3 hours	1.6	102
par32_6	parallel	32	6 hours	2.0	930
par64_1	parallel	64	1 hour	0.1	209
par64_3	parallel	64	3 hours	8.5	55
par64_6	parallel	64	6 hours	17.3	227
par128_1	parallel	128	1 hour	0.9	371
par128_3	parallel	128	3 hours	4.5	90
par128_6	parallel	128	6 hours	2.7	26
par128_12	parallel	128	12 hours	9.5	193
par256_1	parallel	256	1 hour	0.4	156
par256_3	parallel	256	3 hours	0.6	22
par256_6	parallel	256	6 hours	6.1	188
par256_12	parallel	256	12 hours	4.4	237
par512_1	parallel	512	1 hour	0.6	182
par512_3	parallel	512	3 hours	0.2	12
par512_6	parallel	512	6 hours	1.2	22
par512_12	parallel	512	12 hours	0.3	95

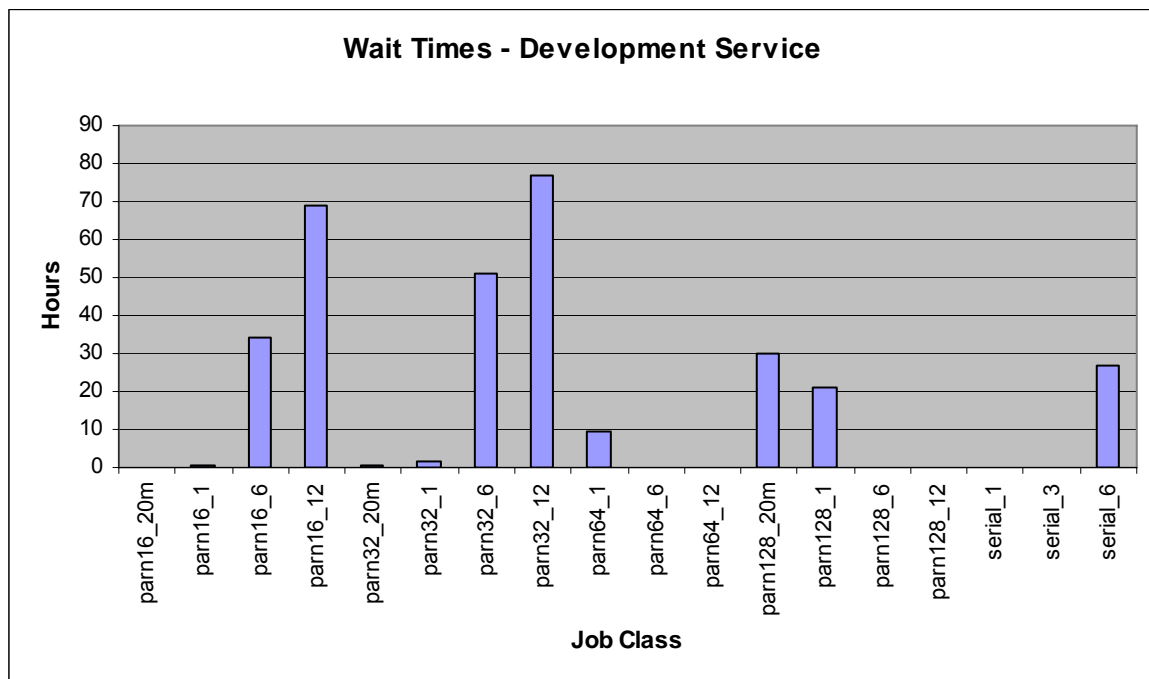
par1024_1	parallel	1024	1 hour	2.5	8
par1024_3	parallel	1024	3 hours	0.0	0
par1024_6	parallel	1024	6 hours	0.0	0
par1024_12	parallel	1024	12 hours	1.2	20
serial_1	serial	1	1 hour	1.3	3747
serial_6	serial	1	6 hours	2.1	167
serial_3	serial	1	3 hours	0.3	25
serial_12	serial	1	12 hours	7.6	214
inter32_1	interactive	32	1 hour	0.0	1123
inter32_20m	interactive	32	20mins	0.0	959
course16_1	parallel	16	1 hour	0.0	0
course32_1	parallel	32	1 hour	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 high utilisation of the service (nearly 88%).

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
inter32_1	interactive	32	1 hour	0.0	199
inter32_20m	interactive	32	20mins	0.0	73
parn128_1	parallel	128	1 hour	20.8	5
parn128_20m	parallel	128	20mins	30.0	2
parn16_1	parallel	16	1 hour	0.8	2123
parn16_12	parallel	16	12 hours	69.0	196
parn16_20m	parallel	16	20mins	0.2	1334
parn16_6	parallel	16	6 hours	34.3	281
parn192_1	parallel	192	1 hour	18.5	1
parn32_1	parallel	32	1 hour	1.5	1157
parn32_12	parallel	32	12 hours	77.0	82
parn32_20m	parallel	32	20 mins	0.7	231
parn32_6	parallel	32	6 hours	51.1	27
parn64_1	parallel	64	1 hour	9.2	71
parn64_20m	parallel	64	20 mins	9.0	23
serial_1	serial	1	1 hour	0.0	3089
serial_12	serial	1	12 hours	0.0	5
serial_3	serial	1	3 hours	0.0	25
serial_6	serial	1	6 hours	26.8	28



2.5 Disk Occupancy

Home Space

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

b02	34,058	50,000
b03	52,711	50,000
b08	21,036	50,000
c01	163,367	300,000
e01	192,009	199,995
e03	62,517	225,012
e05	376,297	665,550
e06	288,513	300,000
e08	93,580	100,000
e10	98,523	150,000
e11	42,777	100,000
e14	74,309	100,000
e15	40,730	50,000
e16	133	20,000
e17	44,927	50,000
e18	37,754	40,000
e19	1,417	40,000
e20	58,105	60,000
e21	1,521	50,000
e22	5,268	10,000
e23	9,733	50,000
e24	63,744	394,376
e25	14,459	50,000
e26	17,033	20,000
e27	19,054	20,000
e29	23,455	50,000
e31	35,459	50,000
e32	47,110	50,000
e33	22,993	50,000
e35	65,216	100,000
e36	49,109	100,000
e37	129,430	204,800
e38	45,722	50,000
e39	105,857	150,000
e40	18,109	50,000
e41	1,532	100,000
e42	65,381	100,000
e44	19	50,000
e45	43,936	50,000
e46	7,105	50,000

e48	5	50,000
e49	39,800	50,000
e50	3,565	13,000
e51	5,181	50,000
e52	11	50,000
e53	13,420	50,000
e54	46,526	50,000
e55	1,664	50,000
e56	47,509	50,000
e58	19,291	100,000
e59	1,348	100,000
e60	17,396	50,000
e61	19,263	50,000
e62	2,255	50,000
n01	107,056	250,000
n02	166,728	299,900
n03	98,558	100,000
n04	192,278	299,999
p01	52,492	200,000
x01	49,190	50,000
x02	8,746	20,000
x03	4,227	50,000
z001	516,686	600,000
z002	89,501	124,000
z004	95,644	100,000
z05	4,188	30,000
z06	64,758	75,000
z07	40,698	50,000
z10	1,980	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	1,335,292	1,349,995
e03	10	500,000
e05	441,656	666,005
e06	367,943	400,000
e08	141	5,000
e10	346,587	400,000
e11	48,527	100,000
e14	121,478	250,000
e15	36,691	100,000

e17	134,939	200,000
e18	51,245	80,000
e19	169,244	200,000
e20	949,980	1,000,000
e21	1	100,000
e23	38,039	100,000
e24	1	2,800,000
e25	142,925	150,000
e27	2,760	40,000
e29	7	9,800
e31	93,144	100,000
e32	99,998	100,000
e33	50,679	100,000
e35	33,762	200,000
e36	50,770	200,000
e37	254,231	307,200
e40	1	100,000
e41	169,046	200,000
e42	353,110	400,000
e48	95,722	200,000
e49	38,704	50,000
e50	180,916	100,000
e53	1,797	150,000
e56	99,999	100,000
e61	24,578	100,000
e62	3,816	200,000
e63	405	200,000
n01	243,073	800,000
n02	7,059,626	8,499,904
n03	24,200	81,002
n04	581,728	750,000
p01	41,764	50,000
x01	158,299	160,000
x03	178	50,000
z001	530,916	600,000
z002	1,617	770
z004	17,601	25,000
z05	4,740	20,000
z06	57,096	100,000
z07	4	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>
n02	6,840,331	9,499,003
n04	6,468	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	70	70	429,774	6,339
e03	5	5	18,797	429
e14	10	10	391,623	595
e15	1	3	26	6
e24	5	12	13,241	913
e26	2	2	545	27
e42	10	10	29,481	447
n01	313	325	35,162	33,686
n02	590	600	772,686	66,593
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

Classifications

<i>Service metric</i>	<i>Number</i>	<i>% of all</i>
Administrative	14	23.3%
Technical	42	70.0%
In-depth	3	5.0%
Technical assessment	0	0.0%
PMR	1	1.7%
<i>Total</i>	60	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 now supply a breakdown of queries by subject category.

<i>Category</i>	<i>Number</i>	<i>% of all</i>
Disks, tapes, resources	16	26.7%
Compilers and system software	16	26.7%
Performance and scaling	4	6.7%
Batch system and queues	4	6.7%
3rd party software	4	6.7%
User behaviour	3	5.0%
Login, passwords, ssh	3	5.0%
User programs	2	3.3%
Access to HPCx	2	3.3%
Tools	1	1.7%
Static website	1	1.7%
Porting	1	1.7%
Other	1	1.7%
None	1	1.7%
Courses	1	1.7%
<i>Total</i>	60	100.0%

Performance

<i>Metric</i>	<i>Achieved</i>	<i>Total</i>	<i>Fraction</i>	<i>Target</i>
Administrative queries - two days	14	14	100%	97%
All queries - three days	53	56	95%	97%
All queries - one day	42	56	75%	75%

Query handlers

<i>Handler</i>	<i>Technical</i>	<i>Admin</i>	<i>In-depth</i>	<i>PMR</i>	<i>Technical assessment</i>
EPCC	15	12	2	0	0
sysadm	12	2	1	1	0
DL	15	0	0	0	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	11.6
Blake	0.8
Bush	16.0
Johnstone	8.0
Jones	1.9
Plummer	10.0
Sunderland	20.0
Todorov	10.0
Total (Days)	78.2
FTEs	4.4

EPCC

<i>Name</i>	<i>Days</i>
Simpson	6.7
Booth	6.4
Henty	10.2
Bull	2.3
Hein	8.0
Jackson	7.2
Reid	10.5
Stratford	4.3
Trew	2.0
Gray	8.6
D'Mellow	12.0
Hill	8.9
Maynard	3.1
Weiland	4.9
Other Staff	15.7
<i>Total (Days)</i>	110.6
<i>FTEs</i>	6.2

Overall Levels

	<i>FTEs</i>
DL	4.4
EPCC	6.2
Total	10.6

4.2 Systems Staffing

<i>Name</i>	<i>Days</i>
Andrews	9.0
Brown	20.0
Fisher	7.5
Georgeson	9.0
Franks	9.0
Jones	1.0
BITD	20.0
Morey	9.0
Kalavsky	14.0
Nazarova	8.2
Total (days)	106.6
FTEs	6.0

Note1: Mr Mike Brown recorded in total over 300 hours for HPCx and HECToR systems support effort during September.

Note2: 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	10.6
Number of training days per month	20/12	25/12	13/9
Non in-depth queries resolved within 3 days	85%	97%	95%
Number of A&M FTEs	3.75	5.75	6.0
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 file systems 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
e62	1	Low Voltage Defibrillation	Dr Vadim Biktashev
e63	1	UKAAC	Dr Nick Hills
e64	1	Jet noise from instability mode interactions	Prof Neil Sandham

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