

HPCx Service Report

March 2007

1 Introduction

This report covers the period from 0800 on 1 March 2007 to 0800 on 1 April 2007. Taking the change to summer time into account, this was a service month of 743 hours.

Overall utilisation of the main service, at nearly 85%, continued to be exceptionally high; the number of AUs delivered this month was another record. There were no SEV1 incidents this month.

2 Usage

2.1 Availability

Incidents

During this month, there were only 4 incidents, none of which was 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	4
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 6.5 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

Consortium	CPU Hours (Parallel)	CPU Hours (Other)	AUs charged	%age of charged AUs
e01	225513	283	1087080	14.8%
e03	2	0	11	0.0%
e05	170686	600	824648	11.2%
e06	17615	75	85169	1.2%
e08	76539	0	368493	5.0%
e10	1172	1	5650	0.1%
e11	11391	0	54840	0.7%
e17	24054	13	115869	1.6%
e21	5277	1	25411	0.3%
e23	18766	0	90347	1.2%
e24	74	0	356	0.0%
e25	0	1	3	0.0%
e26	0	0	0	0.0%
e27	24902	5	111870	1.5%
e32	24553	17	118290	1.6%
e33	12719	0	61237	0.8%
e35	153052	1	736865	10.0%
e36	77	62	666	0.0%
e37	199318	1	959607	13.1%
e38	16	0	75	0.0%
e39	6374	19	30775	0.4%
e40	537	0	2584	0.0%
e41	326	0	1568	0.0%
e42	11081	4	53365	0.7%
e45	6693	0	32224	0.4%
e46	12	0	55	0.0%
e48	692	0	3332	0.0%
e49	125	37	783	0.0%
e50	4249	0	20458	0.3%
e51	644	0	3099	0.0%
e53	0	118	568	0.0%
e54	50836	6	244777	3.3%
<i>EPSRC Total</i>	1077556	1243	5179530	70.6%

n01	29743	10	143247	2.0%
n02	166736	13	802806	10.9%
n03	171594	556	819038	11.2%
n04	34616	271	167962	2.3%
<i>NERC Total</i>	402689	851	1933052	26.3%

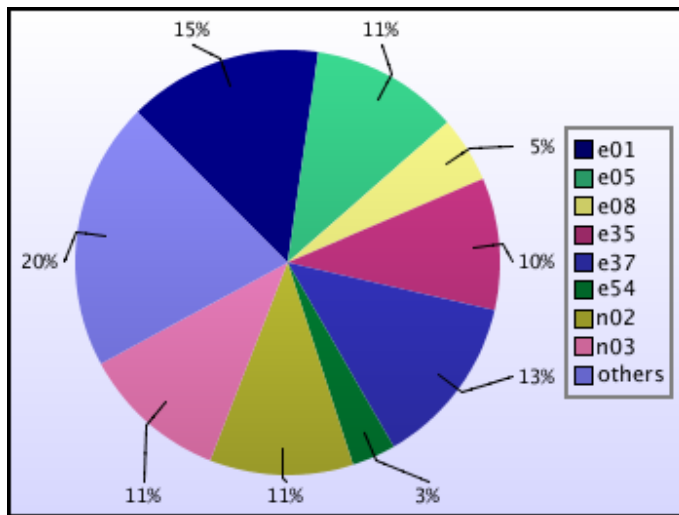
p01	505	0	2433	0.0%
<i>PPARC Total</i>	505	0	2433	0.0%

c01	17894	41	86344	1.2%
<i>CCLRC Total</i>	17894	41	86344	1.2%

b08	20909	1	100669	1.4%
<i>BBSRC Total</i>	20909	1	100669	1.4%

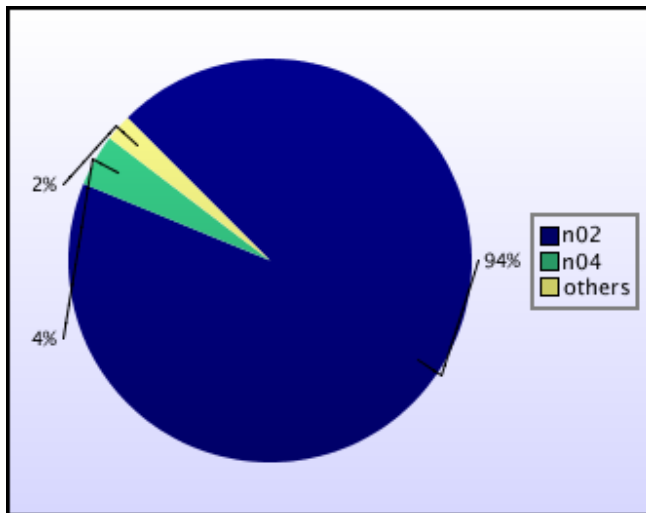
x01	5339	102	26196	0.4%
<i>External Total</i>	5339	102	26196	0.4%

z001	2506	18	12153	0.2%
z004	14	28	199	0.0%
z006	0	0	0	0.0%
<i>HPCx Total</i>	2520	47	12356	0.2%



Development Service

Consortium	CPU Hours (Parallel)	CPU Hours (Other)	AUs charged	%age of charged AUs
n01	1	0	3	0.0%
n02	129507	308	624990	93.7%
n03	2970	0	14300	2.1%
n04	5742	0	27642	4.1%
<i>NERC Total</i>	138220	308	666935	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	882137	12.0%	4490
33–64	467674	6.4%	906
65–128	1462000	19.9%	1310
129–256	3254350	44.3%	685
257–512	727261	9.9%	115
513–1024	560172	7.6%	53
>1024	0	0.0%	0

Overall utilisation of the main service was 84.8%. Capability usage was 17.5% of the total.

Development Service

<i>Number of processors</i>	<i>Raw AUs</i>	<i>%age</i>	<i>Number of jobs</i>
≤32	629036	94.5%	9740
33–64	35798	5.4%	200
65–128	617	0.1%	1
129–256	0	0.0%	0

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:

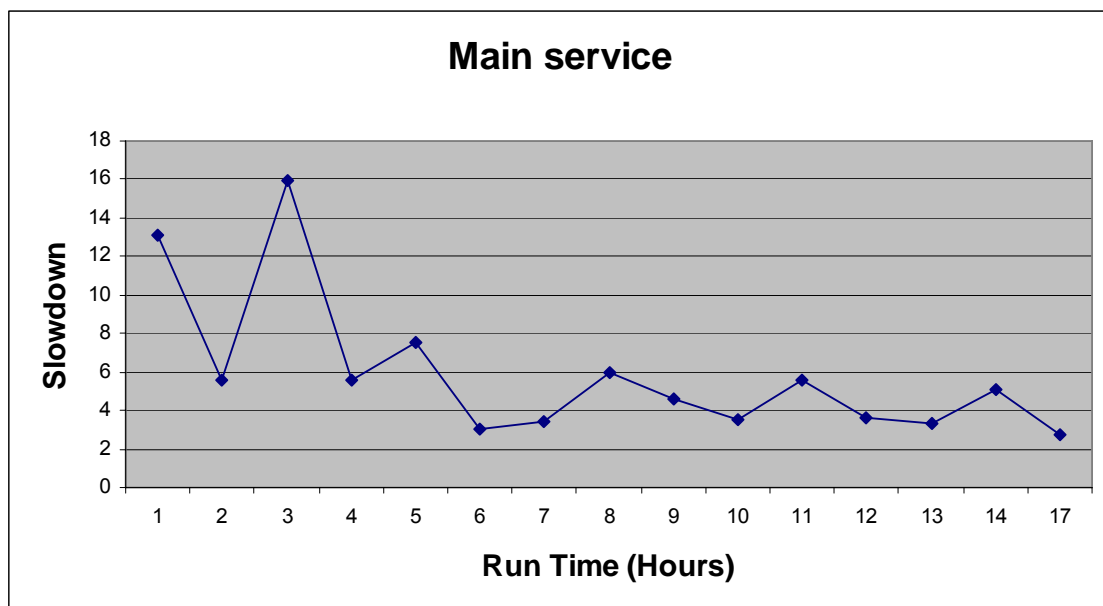
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

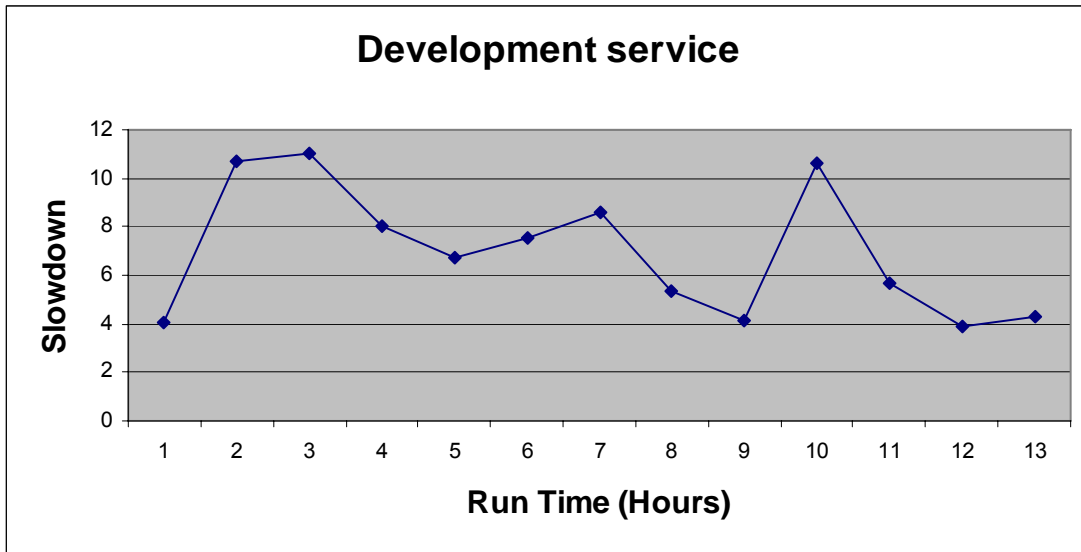
Slowdowns of less than around 10 are usually regarded as reasonable.

On both services, slowdowns are currently generally satisfactory, especially considering the very heavy load on the service.

Slowdowns by runtime

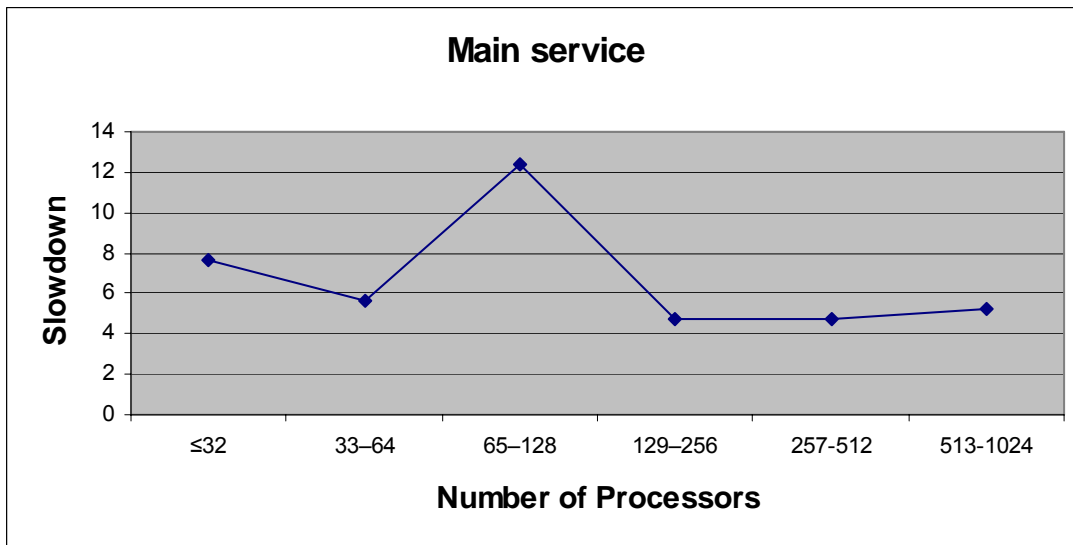
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.



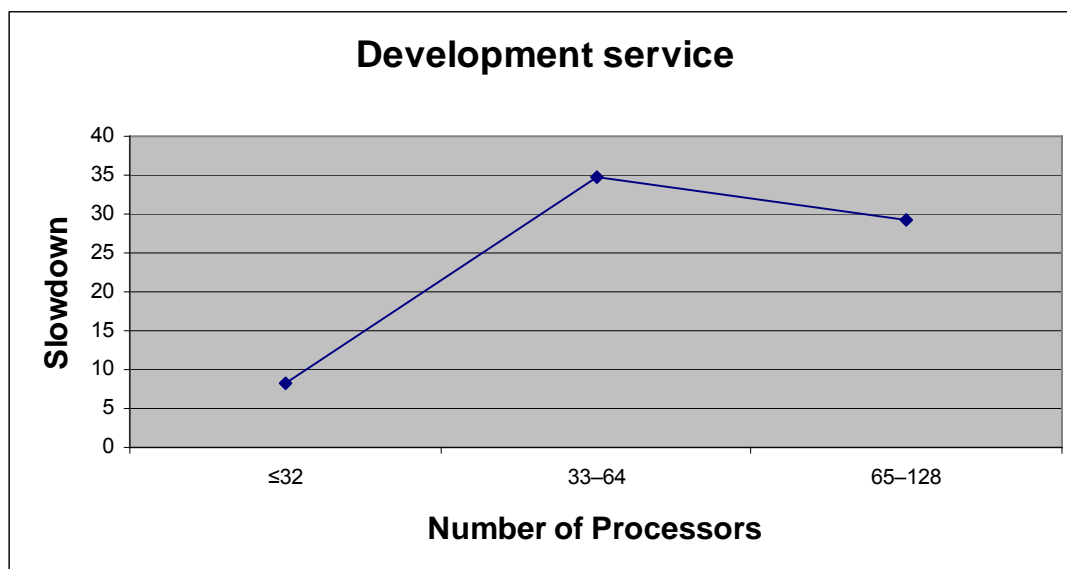


Slowdowns by number of processors

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.



Note that the graph for the development service (see below) summarises 430 jobs at 32 processors or less, 10 at 64 processors and just 1 at 128. The slowdown for the typical job is therefore satisfactory, on a service with extremely high utilisation.

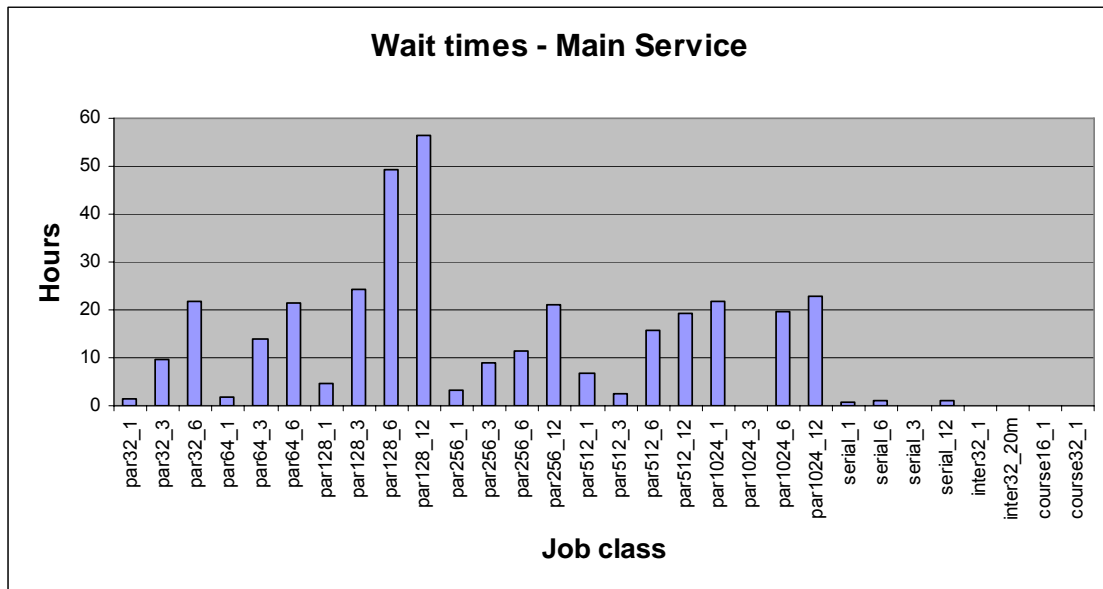


Job wait times – main service

The following table and graph shows the average wait time (in hours) for each class of job on the main service. 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	1.5	2194
par32_3	parallel	32	3	9.6	103
par32_6	parallel	32	6	21.8	2193
par64_1	parallel	64	1	1.9	560
par64_3	parallel	64	3	14.1	46
par64_6	parallel	64	6	21.5	300
par128_1	parallel	128	1	4.5	858
par128_3	parallel	128	3	24.3	35
par128_6	parallel	128	6	49.2	204
par128_12	parallel	128	12	56.5	213
par256_1	parallel	256	1	3.0	143
par256_3	parallel	256	3	9.0	37
par256_6	parallel	256	6	11.3	84
par256_12	parallel	256	12	21.2	421
par512_1	parallel	512	1	6.6	48
par512_3	parallel	512	3	2.6	3
par512_6	parallel	512	6	15.8	4
par512_12	parallel	512	12	19.4	60
par1024_1	parallel	1024	1	21.7	11
par1024_3	parallel	1024	3	0.0	0

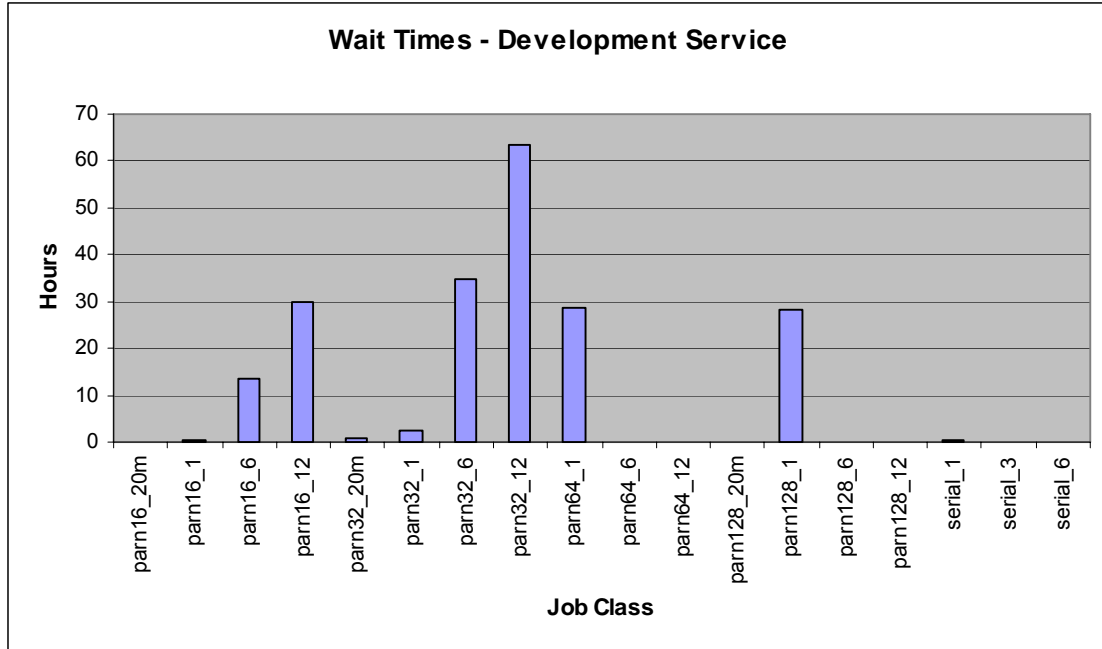
par1024_6	parallel	1024	6	19.5	1
par1024_12	parallel	1024	12	23.0	41
serial_1	serial	1	1	0.7	2652
serial_6	serial	1	6	1.1	303
serial_3	serial	1	3	0.1	67
serial_12	serial	1	12	1.2	143
inter32_1	interactive	32	1	0.0	1895
inter32_20m	interactive	32	1	0.0	1114
course16_1	interactive	16	1	0.0	368
course32_1	parallel	32	1	0.0	58



Job wait times – development service

Job Class	Category	Maximum Number of CPUs	Maximum Job length	Average wait time	Number of Jobs
parn16_20m	parallel	16	20 mins	0.1	3218
parn16_1	parallel	16	1 hour	0.5	4146
parn16_6	parallel	16	6 hours	13.4	96
parn16_12	parallel	16	12 hours	30.0	188
parn32_20m	parallel	32	20 mins	0.8	337
parn32_1	parallel	32	1 hour	2.6	1569
parn32_6	parallel	32	6 hours	34.8	76
parn32_12	parallel	32	12 hours	63.3	110
parn64_1	parallel	64	1 hour	28.6	171
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	28.2	1

parn128_6	parallel	128	6 hours	0.0	0
parn128_12	parallel	128	12 hours	0.0	0
serial_1	serial	1	1 hour	0.2	5691
serial_3	serial	1	12 hours	0.0	26
serial_6	serial	1	12 hours	0.0	1



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	50,000
b03	52711	50,000
b08	44525	50,000
c01	148790	150,000
e01	173122	199,995
e03	59189	225,012
e05	319451	576,050
e06	292953	300,000
e08	95785	100,000
e10	51158	150,000
e11	38262	100,000
e14	98620	100,000
e15	40791	50,000
e16	133	20,000
e17	47086	50,000
e18	32350	40,000
e19	1417	40,000
e20	59001	60,000
e21	1521	50,000
e22	5268	10,000
e23	9733	50,000
e24	126236	394,376
e25	8769	50,000
e26	18320	20,000
e27	19997	20,000
e29	20835	30,000
e30	0	40,000
e31	43633	50,000
e32	47046	50,000
e33	6974	50,000
e34	0	50,000
e35	83420	100,000
e36	49736	50,000
e37	96194	100,000
e38	10042	50,000
e39	22911	150,000
e40	18017	50,000
e41	1521	100,000

e42	26770	100,000
e45	38793	50,000
e46	6579	50,000
e47	0	50,000
e48	5	50,000
e49	25846	50,000
e50	3241	13,000
e51	4469	50,000
e52	11	50,000
e53	1748	50,000
e54	49791	50,000
e55	1664	50,000
e56	47509	50,000
e57	0	50,000
e58	52902	100,000
e60	128	50,000
e61	0	50,000
n01	55590	100,000
n02	165956	298,000
n03	81457	100,000
n04	226916	299,999
p01	42263	200,000
x01	37902	50,000
x02	8746	20,000
x03	4227	50,000
z001	469354	500,000
z002	45259	124,000
z003	0	3
z004	89682	100,000
z05	4188	30,000
z06	57993	75,000
z07	32829	50,000
z10	67	50,000

Workspace

<i>Consortium</i>	<i>Disc Occupancy (Mb)</i>	<i>Disc Quota (Mb)</i>
b02	15	1,025
b03	47908	100,000
b08	5100	50,000
c01	91650	100,000
e01	1131695	1,249,995
e03	10	500,000
e05	359941	623,004
e06	368053	400,000
e08	141	5,000
e10	326252	400,000

e11	42640	100,000
e14	197567	250,000
e15	37597	100,000
e16	0	60,000
e17	93651	100,000
e18	24820	80,000
e19	169244	200,000
e20	941925	1,000,000
e21	1	100,000
e22	0	20,000
e23	37389	100,000
e24	2042838	2,800,000
e25	129673	150,000
e26	0	40,000
e27	2760	40,000
e29	5296	8,000
e30	0	80,000
e31	96130	100,000
e32	99998	100,000
e33	73278	100,000
e34	0	100,000
e35	0	200,000
e36	35655	50,000
e37	94340	150,000
e38	0	100,000
e39	0	100,000
e40	1	100,000
e41	47170	200,000
e42	232904	400,000
e45	0	100,000
e46	0	50,000
e47	0	160,000
e48	99400	200,000
e49	25224	50,000
e50	184589	100,000
e51	0	100,000
e52	0	50,000
e53	684	150,000
e54	0	100,000
e55	0	100,000
e56	99999	100,000
e57	0	100,000
e58	0	200,000
e60	0	100,000
e61	0	100,000
n01	317824	800,000
n02	2171984	2,999,904
n03	18035	81,002

n04	356125	750,000
p01	41764	50,000
x01	131862	160,000
x02	0	20,000
x03	178	50,000
z001	452948	500,000
z002	1617	770
z003	0	3
z004	4577	25,000
z05	4740	20,000
z06	69216	100,000
z07	28	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>
n01	0	500,000
n02	8563091	8,999,003
n04	346217	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	60	60	240433	5893
e03	5	5	18797	429
e14	10	10	391623	595
e15	1	3	26	6
e24	10	10	14459	1524
e26	2	2	545	27
e42	10	10	29481	447
n01	291	295	32453	31569
n02	383	410	475519	42046
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	105	67.7
Technical	40	25.8
In-depth	9	5.8
PMR	1	0.6
TOTAL	155	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 3 platform	95	61.3
Website	1	0.6
Other/general	59	38.1
TOTAL	155	100.0

Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	130	89.7	75%
Finished within 72 Hours	145	100.0	97%
Finished after 72 Hours	0	0.0	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	103	98.1	97%
Finished after 48 Hours	2	1.9	

Experts Handling Queries

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	90	15	6	0
dl.ac.uk	4	11	0	1
Sysadm	11	14	3	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>
HPC Techniques in Computational Chemistry	06-Mar	3	25	18	0

4 Staffing

4.1 Science Support Staffing

Daresbury Laboratory

<i>Name</i>	<i>Days</i>
Ashworth	15.4
Blake	2.2
Bush	22.0
Guest	5.5
Johnstone	6.6
Plummer	11.0
Sunderland	22.0
Total (Days)	84.7
FTEs	4.8

EPCC

<i>Name</i>	<i>Days</i>
Simpson	15.8
Booth	14.2
Henty	8.7
Smith	12.5
Bull	9.2
Fisher	5.0
Hein	19.5
Jackson	1.7
Reid	8.8
Stratford	9.8
Nazarova	12.6
Trew	4.3
Gray	6.9
D'Mellow	11.3
Hill	0.5
Johnson	0.9
Maynard	2.0
Weiland	21.1

Other staff	0.5
Total (Days)	165.0
FTEs	9.3

Overall Levels

	<i>FTEs</i>
DL	4.8
EPCC	9.3
Total	14.1

4.2 Systems Staffing

<i>Name</i>	<i>Days</i>
Andrews	17.6
Brown	21.0
Fisher	10.5
Georgeson	16.0
Franks	17.6
Jones	3.0
BITD	17.6
Total (Days)	103.3
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%	100.0%
Technology MTBF (hours)	200	300	∞
Number of AV FTEs	7.5	10	14.1
Number of training days per month	20/12	25/12	7/3
Non in-depth queries resolved within 3 days	85%	97%	100.0%
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>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 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
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
e57	1	Triplex DNA Structures	Dr Hooshang Nikjoo

e58	1	Quantum Simulations for Chemical Biology	Dr Carmen Domene
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