

HPCx Quarterly Report

October - December 2004

1 Introduction

This report covers the period from 1 October 2004 at 0800 to 1 January 2005 at 0800.

The next section summarises the main points of the service for this quarter. Section 3 gives details of the usage of the service, including failures, serviceability, CPU usage, helpdesk statistics and service quality tokens. A summary table of the key performance metrics is given in the final section. The Appendices define the incident severity levels and list the current HPCx projects.

2 Executive Summary

- There were only 3 failures this quarter and none of these were directly related to failures of the hardware. Correspondingly, the serviceability and MTBF figures have been very good. The Phase 2 system has become stable much earlier than expected and has so far proven to be very reliable.
- The usage of the production region and the capability usage were disappointing during this quarter. A report on this, including strategies for improving capability utilisation, has been prepared for the forthcoming meeting of the Oversight Committee.
- HPCx have provided additional support for BBSRC consortia (through the Life Science Initiative) and NERC consortia (via a users' workshop); subsequently, usage from both BBSRC and NERC has been higher during the last few months of the year.
- The helpdesk again met all the targets for queries during this quarter.
- The target for training days was completed by running two courses remotely at the Rutherford Appleton Laboratory. These courses were on *Optimisation* and *Performance Scaling* and had good turnouts from HPCx users.

- The Terascaling team have reported good performance improvements for a variety of codes, including a 50% improvement for the CENTORI fusion code from Culham.
- NCAS (n02) use SRB (Storage Resource Broker) to manage their datasets; at their request, we have now installed the SRB client toolkit to allow users to access remote SRB data repositories from HPCx.
- HPCx was publicised at SC2004 by a display on the joint EPCC-Daresbury booth, a presentation at the IBM booth and a tutorial on *Improved Performance Scaling*.
- We provided support for a number of bids to the Call for Proposals for joint experiments with TeraGrid to follow on from the success of TeraGyroid.

3 Usage Statistics

3.1 Availability

3.1.1 Failures

The monthly numbers of incidents and failures (SEV 1 incidents) are shown in the table below:

	<i>October</i>	<i>November</i>	<i>December</i>
Incidents	15	11	12
Failures	0	2	1

The following tables give more details on the attribution of the failures:

October

There were no failures.

November

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
04.235	0%	0%	100%	Manchester network problem
04.239	50%	50%	0%	Maintenance session overrun

December

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
04.253	100%	0%	0%	Networking problem disabled website

3.1.2 Performance Statistics

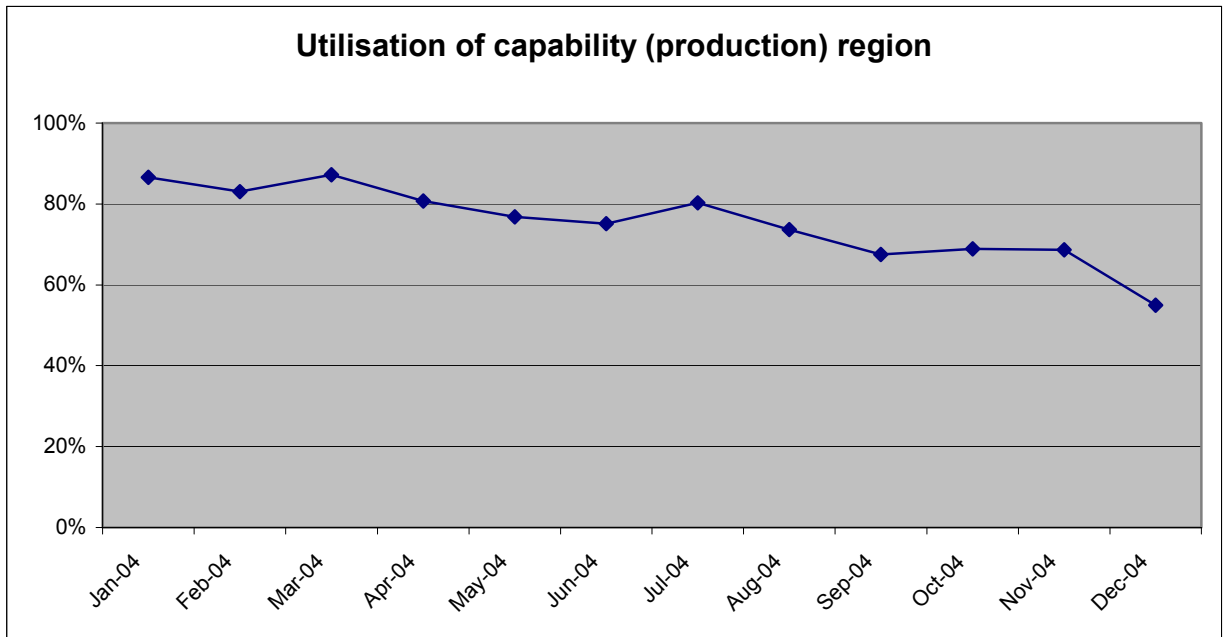
This section uses the definitions agreed in Schedule 7, ie,

- $MTBF = (24 \times 30.5) / (\text{number of failures in month})$
- $\text{Serviceability (\%)} = 100 \times (\text{WCT} - \text{SDT} - \text{UDT}) / (\text{WCT} - \text{SDT})$

<i>Attribution</i>	<i>Metric</i>	<i>October</i>	<i>November</i>	<i>December</i>	<i>Quarterly</i>
IBM	Failures	0	0.5	0	0.5
	MTBF	∞	1464	∞	4392
	Serviceability	100.0%	99.9%	100.0%	99.9%
Site	Failures	0	0.5	1	1.5
	MTBF	∞	1464	732	1464
	Serviceability	100.0%	99.9%	97.8%	99.9%
External	Failures	0	1	0	1
	MTBF	∞	732	∞	2196
	Serviceability	100.0%	99.8%	100.0%	99.9%
Total	Failures	0	2	1	3
	MTBF	∞	366	732	732
	Serviceability	100.0%	99.5%	97.8%	99.9%

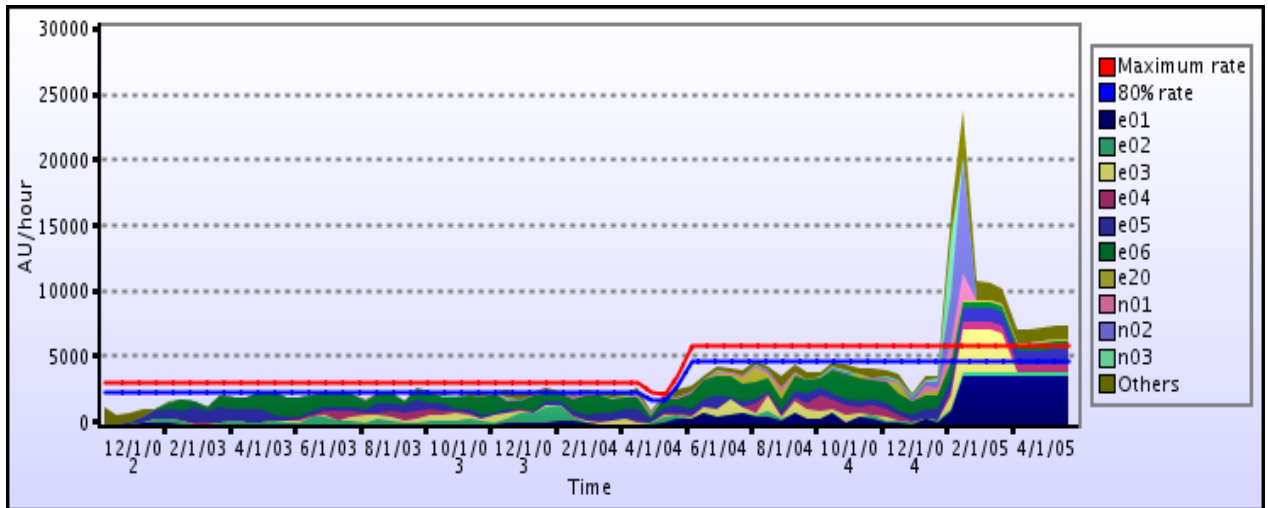
3.2 Capability Utilisation

The monthly utilisation for the production region is shown in the graph below. This has averaged around 65% for this quarter, which is clearly disappointing given the previous values.



3.3 Capacity Planning

Predicted Utilisation



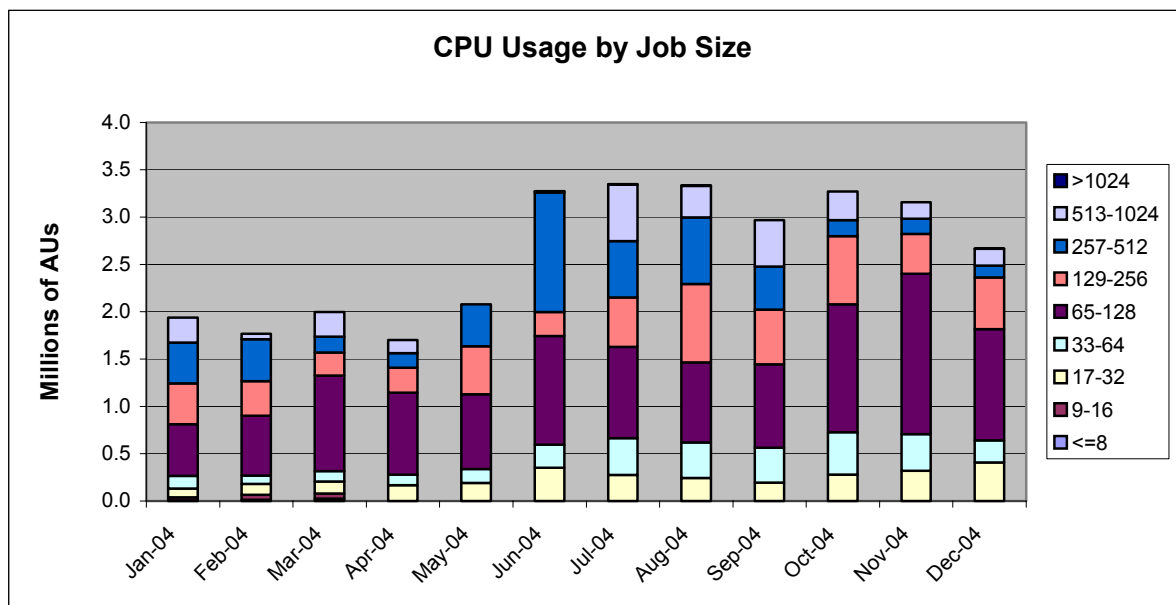
The graph above shows the utilisation since the start of the project and the projected utilisation until May 2005. The scale on the y-axis is AU per hour, where the peak that HPCx Phase 1 could currently deliver is around 3240 AUs per hour, and Phase 2 6188 AUs per hour (the upper red line in the graph). The lower line (in blue) corresponds to the more practicable 80% level.

The graph assumes that each project will use its remaining allocation pro rata with its usage profile from the SAF, which is often simply that on the original application form.

Numbers of Research Consortia

There are currently 36 research consortia using the HPCx system. Three other projects have now been closed. In addition, there is one externally-funded project and a project performing preparatory benchmarking work for the HECToR procurement.

3.4 CPU Usage by Job Size



3.5 AU Usage by Consortium

The PIs and titles for the various consortia are listed in Appendix B.

<i>Consortium</i>	<i>October</i>	<i>November</i>	<i>December</i>	<i>Quarterly</i>	<i>%age</i>
e01	495363	355578	161786	1012727	11.1%
e02	1115	70622	58141	129878	1.4%
e03	346706	177303	71899	595908	6.5%
e04	641661	495523	329296	1466480	16.1%
e05	380140	274012	285786	939938	10.3%
e06	937164	1301361	991717	3230242	35.4%
e07	26044	11743	8862	46649	0.5%
e08	1280	8110	240	9630	0.1%
e10	37843	4176		42019	0.5%
e11	13395	102445	60768	176608	1.9%
e15	124		618	742	0.0%
e17		2790	4093	6883	0.1%
e18		13040		13040	0.1%
e20	19744	73368	269732	362844	4.0%
e24	524	793		1317	0.0%
z09			4192	4192	0.0%
<i>EPSRC Total</i>	2901102	2890864	2247130	8039096	88.2%

n01	839	13117	37642	51598	0.6%
n02	70048	48961	139072	258081	2.8%
n03	121953	20023	18589	160565	1.8%
n04	75277	19775	47015	142067	1.6%
<i>NERC Total</i>	268116	101877	242318	612311	6.7%

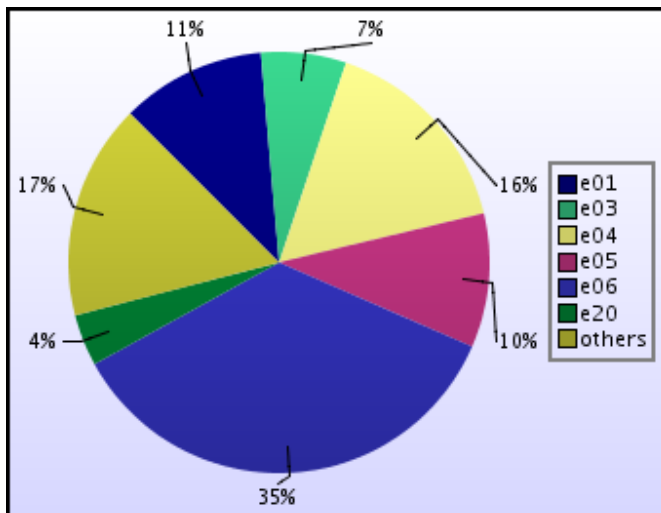
p01	3213	16266	4955	24434	0.3%
<i>PPARC Total</i>	3213	16266	4955	24434	0.3%

c01	25487	51281	51090	127858	1.4%
<i>CCLRC Total</i>	25487	51281	51090	127858	1.4%

b02		23123	8944	32067	0.4%
b05			34092	34092	0.4%
b07	1	5464	5	5470	0.1%
<i>BBSRC Total</i>	1	28587	43040	71628	0.8%

x01	53505	31117	39857	124479	1.4%
<i>External Total</i>	53505	31117	39857	124479	1.4%

z001	22193	47583	42413	112189	1.2%
z002		488	49	537	0.0%
z004	18	20		38	0.0%
z05		0	263	263	0.0%
z06	737	969	953	2659	0.0%
<i>HPCx Total</i>	22948	49060	43679	115687	1.3%



3.5.1 Discounts

There are now a number of user codes that have qualified for capability discounts. The following table shows the discounts that were awarded during the last quarter.

<i>Consortium</i>	<i>AUs Used</i>	<i>AUs Charged</i>	<i>Discount</i>
b05	36894	34091	2803

3.6 Helpdesk

3.6.1 Classifications

<i>Category</i>	<i>Number</i>	<i>% of all</i>
Administrative	140	49.6
Technical	120	42.6
In-depth	19	6.7
PMR	3	1.1
TOTAL	282	100.0

<i>Service Area</i>	<i>Number</i>	<i>% of all</i>
Phase 1/2 platforms	199	70.6
Website	17	6.0
Other/general	66	23.4
TOTAL	282	100.0

3.6.2 Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	208	80.0	75%
Finished within 72 Hours	258	99.2	97%
Finished after 72 Hours	2	0.8	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	140	100.0	97%
Finished after 48 Hours	0	0.0	

3.6.3 Experts Handling Queries

<i>Expert</i>	<i>Admin</i>	<i>Technical</i>	<i>In-Depth</i>	<i>PMR</i>
epcc.ed.ac.uk	116	64	7	1
dl.ac.uk	6	21	5	0
Sysadm	18	35	7	2
Other people	0	0	0	0

3.7 Service Quality Tokens

<i>Date</i>	<i>Person</i>	<i>Value</i>	<i>Comment</i>	<i>Status</i>
Dec 24, 2004 9:05:47 PM	Dr Abdulnaser I Sayma	* * *		

4 Support

Details of the current status of science support can be found in the *HPCx Annual Report: 2004*.

4.1 Staffing

AV	October	November	December
DL	5.7	5.4	5.0
EPCC	8.3	8.7	5.3
Total	14.0	14.2	10.3

Systems	4.9	6.6	5.4
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5 Summary of Performance Metrics

<i>Metric</i>	<i>TSL</i>	<i>FSL</i>	<i>October</i>	<i>November</i>	<i>December</i>
Technology serviceability	80%	99.2%	100.0%	99.9%	100.0%
Technology MTBF (hours)	200	300	∞	1464	∞
Number of AV FTEs	7.5	10	14.0	14.2	10.3
Number of training days per month	22.5/12	30/12	28/10	30/11	30/12
Non in-depth queries resolved within 3 days	85%	97%	100.0%	98.6%	97.7%
Number of A&M FTEs	3.75	5.75	4.9	6.6	5.4
A&M serviceability	80%	99.6%	100.0%	99.9%	97.8%

<i>Colour</i>	<i>Meaning</i>
	Exceeds FSL
	Between TSL and FSL
	Below TSL

Note 1: The number of training days is reported as a running total since the start of the year.

Note 2: The above table includes the revised FSL targets for *training days* and *A&M serviceability*, which have been provisionally agreed with EPSRC.

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	Prof Neil Sandham
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
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
e12	1	Parallel programs for the simulation of complex fluids	Dr Mark R Wilson
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
z09		HECToR Benchmarking	Dr Edward Smyth

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
n05	2	Non-linear Wave-particle Instabilities in Plasmas	Dr Mervyn Freeman

BBSRC Projects

<i>Code</i>	<i>Class</i>	<i>Title</i>	<i>PI</i>
b02	1	Modelling enzyme catalysis	Dr Adrian J Mulholland
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
b07	1	Simulation of Radioprobing	Dr Charlie Laughton

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

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
e09	2	Molecular Properties and their Geometry	Prof Peter Taylor
e13	1	TeraGyroid project	Dr Richard J Blake