

# **HPCx Quarterly Report**

## **October - December 2005**

### **1 Introduction**

This report covers the period from 1 October 2005 at 0800 to 1 January 2006 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**

- The Phase 2A upgrade to Power 5 technology went well with less than 48 hours downtime to switch over the service. This was the result of careful planning and hard work by both IBM and the HPCx Systems team. While there were a number of failures subsequent to the upgrade, we are confident that these were due to teething problems that have now been resolved.
- Usage on the system has remained high throughout the quarter; October was a record month for both utilisation and total AUs delivered. This has also been an excellent quarter for capability usage with both November and December being record months. In fact, December was the first month of the service where capability usage exceeded 50%.
- Usage by NERC users has been consistently high this quarter and usage by BBSRC users was particularly high in December.
- Only 1% of the non-indepth queries took longer than the allowed 72 hours.
- The target for training days was met by running five different courses this quarter, including a number of new or updated courses.

- The number of consortia remains high and we expect to be at or above the maximum of 40 during 1Q06; we will continue to monitor this over the next few months.
- QinetiQ completed a security audit of the HPCx system, which identified a number of issues, although the overall security level was good. This was followed by an internal security re-assessment in light of the findings.
- HPCx had a significant presence at SC05 where we had a display, coordinated between the EPCC and Daresbury research booths, which highlighted the capability science being done in the UK. We provided significant support for the SPICE project that won the HPC Analytics Challenge.
- We also ran a well-attended workshop on Environmental Engineering during November, which was aimed at raising awareness of the potential benefits of using the UK's high-end computing facilities and stimulating discussion between leading research groups in this broad area.
- The HPCx Annual Seminar on *Capability Science on HPCx* was run at Daresbury, immediately before the Annual Machine Evaluation Workshop, and attracted a good audience. The final session included an HPCx User Group meeting.

### 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	19	10	13
Failures	1	1	5

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

##### *October*

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
05.142	0%	0%	100%	Loss of external network

##### *November*

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
05.156	100%	0%	0%	16 nodes locked by memory overflow

##### *December*

<i>Failure</i>	<i>Site</i>	<i>IBM</i>	<i>External</i>	<i>Reason</i>
05.158	0%	100%	0%	GPFS failure on /hpcx/home
05.159	0%	100%	0%	GPFS failure on /hpcx/home
05.162	100%	0%	0%	Site firewall failure
05.163	100%	0%	0%	Site firewall failure
05.164	100%	0%	0%	Capability region drained in error

### 3.1.2 Performance Statistics

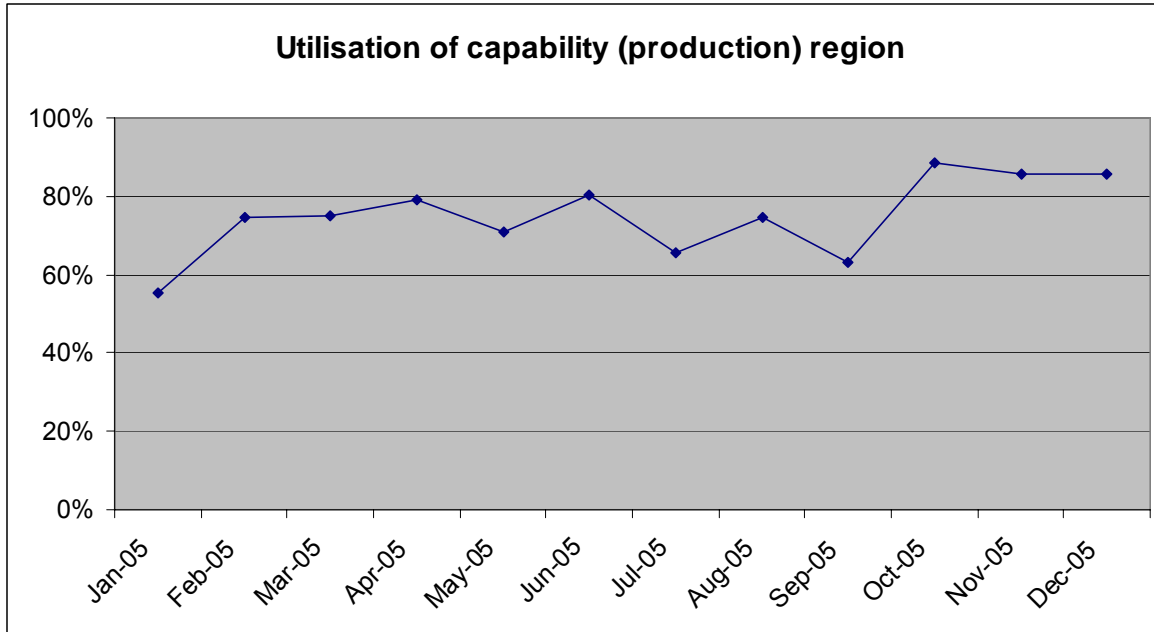
This section uses the definitions agreed in Schedule 7, ie,

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

<i>Attribution</i>	<i>Metric</i>	<i>October</i>	<i>November</i>	<i>December</i>	<i>Quarterly</i>
IBM	Failures	0	0	2	2
	MTBF	∞	∞	366	1098.0
	Serviceability	100.0%	100.0%	98.3%	99.4%
Site	Failures	0	1	3	4
	MTBF	∞	732	244	549.0
	Serviceability	100.0%	99.5%	97.7%	99.0%
External	Failures	1	0	0	1
	MTBF	732	∞	∞	2196.0
	Serviceability	100.0%	100.0%	100.0%	100.0%
Total	Failures	1	1	5	7
	MTBF	732	732	146	313.7
	Serviceability	100.0%	99.5%	95.9%	98.4%

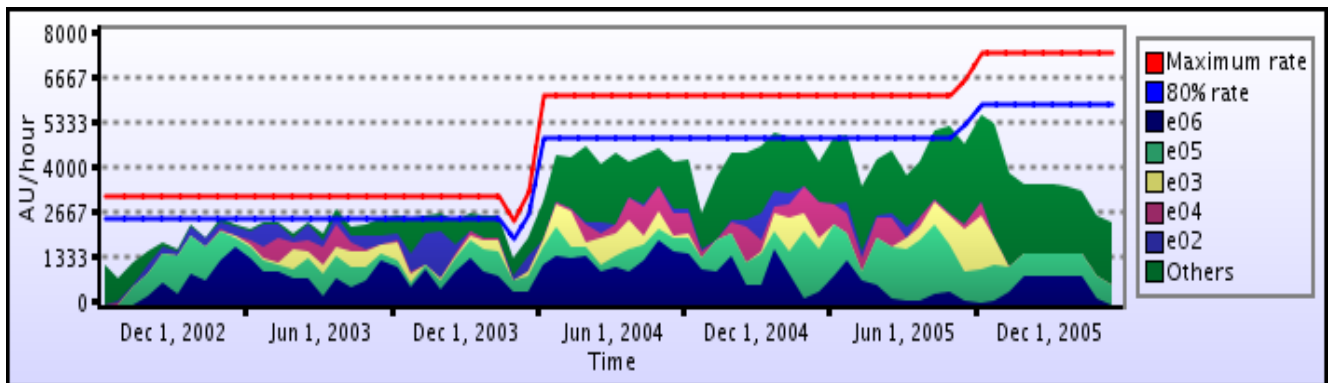
### 3.2 Capability Utilisation

The monthly utilisation for the production region (the capability region on Phase 2A) is shown in the graph below. This has averaged around 86.5% for the quarter, making it the busiest quarter in the service so far.



### 3.3 Capacity Planning

#### *Predicted Utilisation*



The graph above shows the utilisation since the start of the project and the projected utilisation until May 2006. The scale on the y-axis is AUs 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

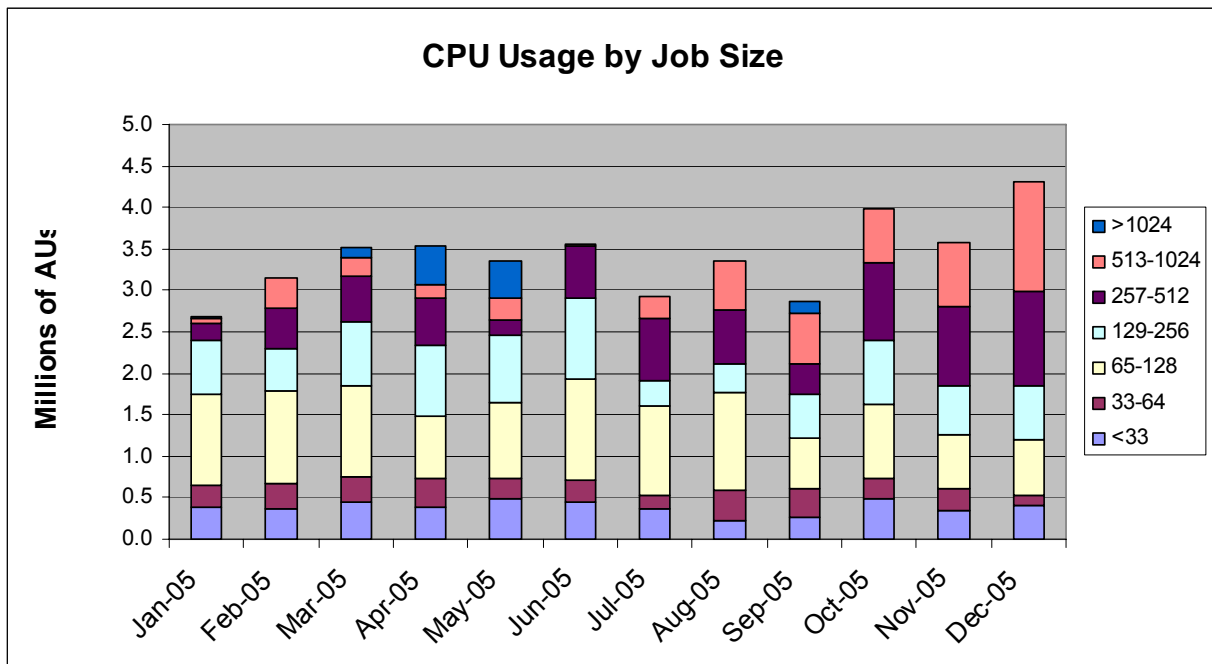
- that each project will use its remaining allocation pro rata with its usage profile from the SAF, which is often simply that on the original application form.;
- that no more projects are given access to the service.

### Numbers of Research Consortia

There are currently 36 research consortia using the HPCx system, with a further nine awaiting access, either immediately or in the first quarter of 2006. Four of the existing consortia have passed their end-dates, and we are awaiting confirmation from the research councils that they should be closed. We thus expect more than 40 consortia on the system by March.

In addition, there is one active 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.

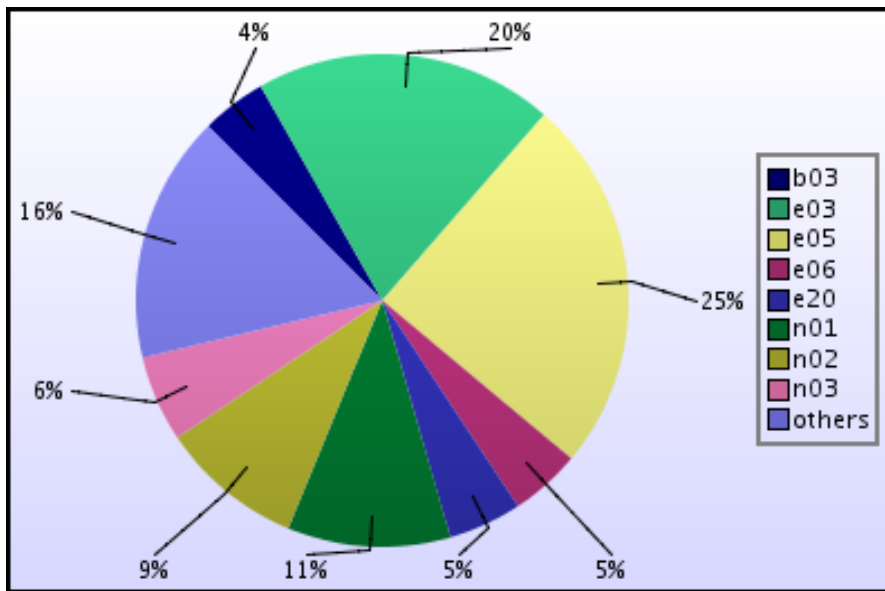
<i>Consortium</i>	<i>October</i>	<i>November</i>	<i>December</i>	<i>Quarterly</i>	<i>%age</i>
e03	522302	808120	921055	2251477	19.6%
e04	36494	60295	166613	263402	2.3%
e05	1398584	718702	712989	2830275	24.7%
e06	188986	229161	113129	531276	4.6%
e07			539	539	0.0%
e08	12808	24164	15372	52343	0.5%
e10	42390	493	2389	45273	0.4%
e11		2960	108883	111843	1.0%
e14	63672	59191	199755	322619	2.8%
e15		197		197	0.0%
e17	23886	72830	31824	128540	1.1%
e18	42669	10036		52706	0.5%
e19		40204		40204	0.4%
e20	197195	197962	158845	554002	4.8%
e24	1320	1271	207	2798	0.0%
e25	1997	1650	5535	9182	0.1%
e26	8	1863	2905	4776	0.0%
e27	1280	22376	0	23656	0.2%
e28	19240	3908	17	23165	0.2%
e29		2900		2900	0.0%
e31	217	31	4615	4863	0.0%
e32		22905		22905	0.2%
e33			100	100	0.0%
z09		12567		12567	0.1%
<i>EPSRC Total</i>	2553049	2293788	2444770	7291607	63.6%
n01	569708	422913	233793	1226414	10.7%
n02	395295	369,813	313193	1078301	9.4%
n03	167188	222532	259334	649054	5.7%
n04	5937	31258	7353	44548	0.4%
<i>NERC Total</i>	1138128	1019650	813673	2998317	26.1%
p01	4219	4832	121	9171	0.1%
<i>PPARC Total</i>	4219	4832	121	9171	0.1%
c01	38640	83156	30242	152038	1.3%

<i>CCLRC Total</i>	38640	83156	30242	152038	1.3%
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b02	25547	18417	235742	279706	2.4%
b03			492022	492022	4.3%
<i>BBSRC Total</i>	25547	18417	727764	771728	6.7%

x01	7880	2048	66623	76551	0.7%
<i>External Total</i>	7880	2048	66623	76551	0.7%

z001	23326	75807	64637	163770	1.4%
z002	1	263	1263	1527	0.0%
z004	1263	5	7	1275	0.0%
z06	607	7190	24	7821	0.1%
<i>HPCx Total</i>	25196	83266	65930	174393	1.5%



### 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>
b02	313892	279705	34186
e04	281752	263401	18351
e05	3096884	2830275	266609
e06	552828	531275	21552
n03	730228	649053	81174

## 3.6 Helpdesk

### 3.6.1 Classifications

<i>Category</i>	<i>Number</i>	<i>% of all</i>
Administrative	145	44.6
Technical	160	49.2
In-depth	19	5.8
PMR	1	0.3
TOTAL	325	100.0

<i>Service Area</i>	<i>Number</i>	<i>% of all</i>
Phase 1/2 platforms	278	85.5
Website	17	5.2
Other/general	30	9.2
TOTAL	325	100.0

### 3.6.2 Performance

<i>All non-indepth queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 24 Hours	262	85.9	75%
Finished within 72 Hours	302	99.0	97%
Finished after 72 Hours	3	1.0	

<i>Administrative queries</i>	<i>Number</i>	<i>%</i>	<i>Target</i>
Finished within 48 Hours	139	95.9	97%
Finished after 48 Hours	6	4.1	

### 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	112	68	13	0
dl.ac.uk	2	23	1	1
Sysadm	29	69	5	0
Other people	2	0	0	0

### 3.7 Service Quality Tokens

<i>Date</i>	<i>Person</i>	<i>Value</i>	<i>Comment</i>	<i>Status</i>
Oct 19, 2005 11:45:58 PM	<a href="#">Dr Dario Alfe</a>	****	[no comment was made]	

## 4 Support

Details of the current status of science support can be found in the *HPCx Annual Report: 2005*.

### 4.1 Staffing

<i>AV</i>	<i>October</i>	<i>November</i>	<i>December</i>
DL	6.6	6.1	4.8
EPCC	9.8	13.2	7.1
Total	16.4	19.4	11.9

<i>Systems</i>	16.4	19.4	11.9
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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%	100.0%	98.3%
Technology MTBF (hours)	200	300	∞	∞	366
Number of AV FTEs	7.5	10	16.4	19.4	11.9
Number of training days per month	22.5/12	30/12	24/10	29/11	30/12
Non in-depth queries resolved within 3 days	85%	97%	98.9%	100.0%	97.2%
Number of A&M FTEs	3.75	5.75	6.0	6.7	5.4
A&M serviceability	80%	99.6%	100.0%	99.5%	97.7%

<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>
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
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

e28	1	Towards the Dynome	Dr Jonathan W Essex
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
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
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

## 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
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
e01	1	UK Turbulence Consortium	Prof Neil Sandham
e09	2	Molecular Properties and their Geometry	Prof Peter Taylor
e12	1	Parallel programs for the simulation of complex fluids	Dr Mark R Wilson
e13	1	TeraGyroid project	Dr Richard J Blake
x02		OHM Ltd	Mr Mark Westwood