HPCx Service Report
August 2005

1 Introduction

This report covers the period from **01/08/2005** at 0800 to **01/09/2005** at 0800. This is a service month of **744** hours.

During August, there were three courses run for a total of 7 training days; this brings us back on target. This month we delivered more than 3.3 million AUs to users, representing a utilisation of around 75%.

1.1 Availability

Incidents

During this month, there were 9 incidents, only one of which was at SEV 1. The following table indicates the severity levels of the incidents, where SEV 1 is defined as a *Failure* (in contractual terms). The definitions used for severity levels can be found in Appendix A.

Severity	*Number*
1	1
2	5
3	3
4	0

The attributions for the SEV 1 incident were as follows:

SEV1	*Incidents*	*MTBF*
IBM	0.0	∞
Site	1.0	732
External	0.0	∞
Overall	1.0	732

The following table gives more details on the Severity 1 incident:

Failure	*Site*	*IBM*	*External*	*Reason*
05.119	100%	0%	0%	Network firewall is a site responsibility

Serviceability

There was a total of 4.9 hours of scheduled downtime this month.

Attribution	*UDT*	*Serviceability*
IBM	0:00	100.0
Site	6:25	99.1
External	0:00	100.0
Overall	6:25	99.1

1.2 CPU Usage by Consortium

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

Consortium	*CPU Hours (Parallel)*	*CPU Hours (Other)*	*AUs charged*	*%age*
e02	22292	457	87980	2.7%
e03	224	25	963	0.0%
e04	158436	17	612817	18.6%
e05	312085	343	1152764	35.0%
e06	70842	35	274118	8.3%
e07	1	0	2	0.0%
e08	2132	0	8247	0.3%
e10	0	0	1	0.0%
e11	978	1	3784	0.1%
e14	2483	67	9862	0.3%
e15	188	0	727	0.0%
e17	1362	0	5269	0.2%
e18	7274	0	28131	0.9%
e19	11746	0	45429	1.4%
e20	11506	55	44712	1.4%
e24	3379	2	13077	0.4%
e25	0	8	31	0.0%
e26	637	3	2473	0.1%
e27	41	0	159	0.0%
e28	5426	6	21008	0.6%

e29	0	0	1	0.0%
e31	964	2	3737	0.1%
z09	16474	0	63713	1.9%
EPSRC Total	628470	1021	2379003	72.2%

n01	68165	20	263707	8.0%
n02	85544	11	330883	10.0%
n03	29077	0	112457	3.4%
n04	5316	17	20627	0.6%
NERC Total	188103	48	727673	22.1%

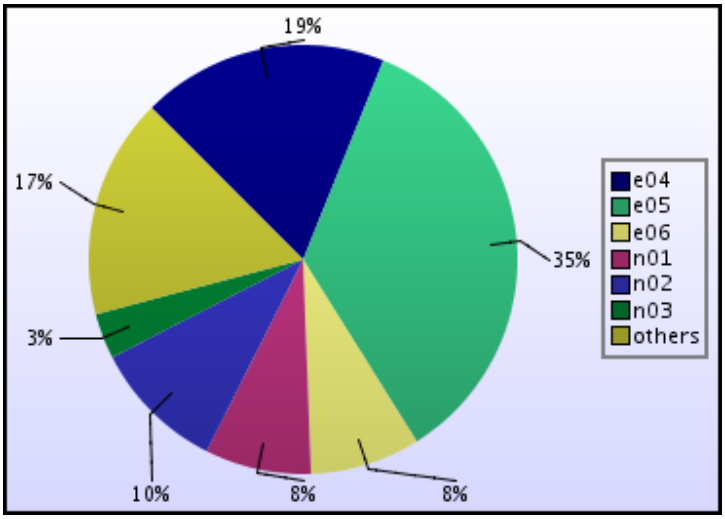
p01	2	0	6	0.0%
PPARC Total	2	0	6	0.0%

c01	15561	371	61614	1.9%
CCLRC Total	15561	371	61614	1.9%

b02	1	0	4	0.0%
b03	10020	0	38751	1.2%
BBSRC Total	10021	0	38756	1.2%

x01	3685	0	14252	0.4%
External Total	3685	0	14252	0.4%

z001	14582	40	56550	1.7%
z004	3983	41	15562	0.5%
z06	106	5	430	0.0%
HPCx Total	18671	86	72542	2.2%



1.3 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. It uses the conversion rate for the AU which corresponds to the results of the Linpack benchmark running on the new platform; that is, 1 CPU hour = 3.8675 AUs.

Number of processors	*Raw AUs*	*%age*	*Number of jobs*
≤32	230063	6.9%	2973
33–64	367739	11.0%	774
65–128	1169791	35.0%	795
129–256	330781	9.9%	355
257–512	665050	19.9%	127
513–1024	577964	17.3%	50
>1024	2114	0.1%	4

The system is divided into three regions.

Development Region (9 frames, jobs using ≤64 CPUs): a total of 597801 raw AUs were used; that is 72.1% of the total available in this region

Production Region (40 frames, jobs using >64 CPUs): a total of 2745700 raw AUs were used; that is 74.5% of the total available in this region

The remaining frame is reserved for interactive parallel jobs.

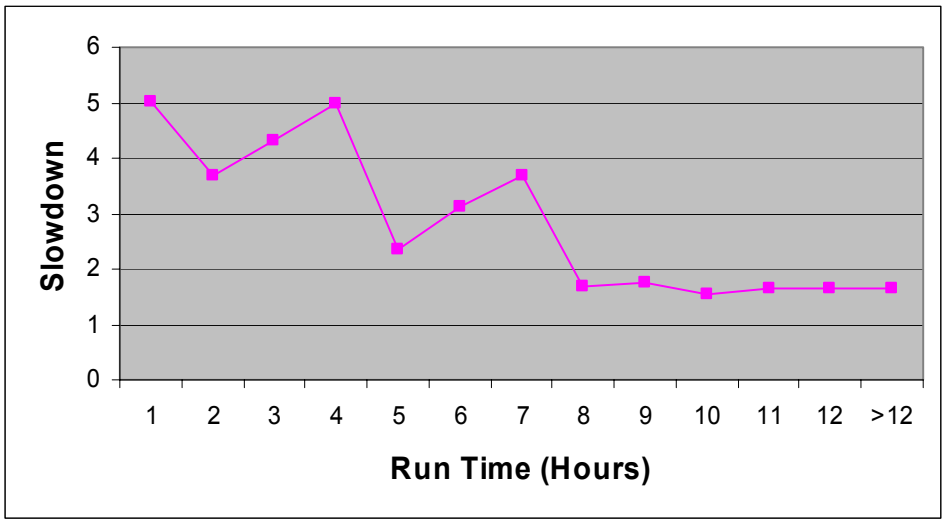
1.4 Slowdown and Job Wait Times

Slowdown

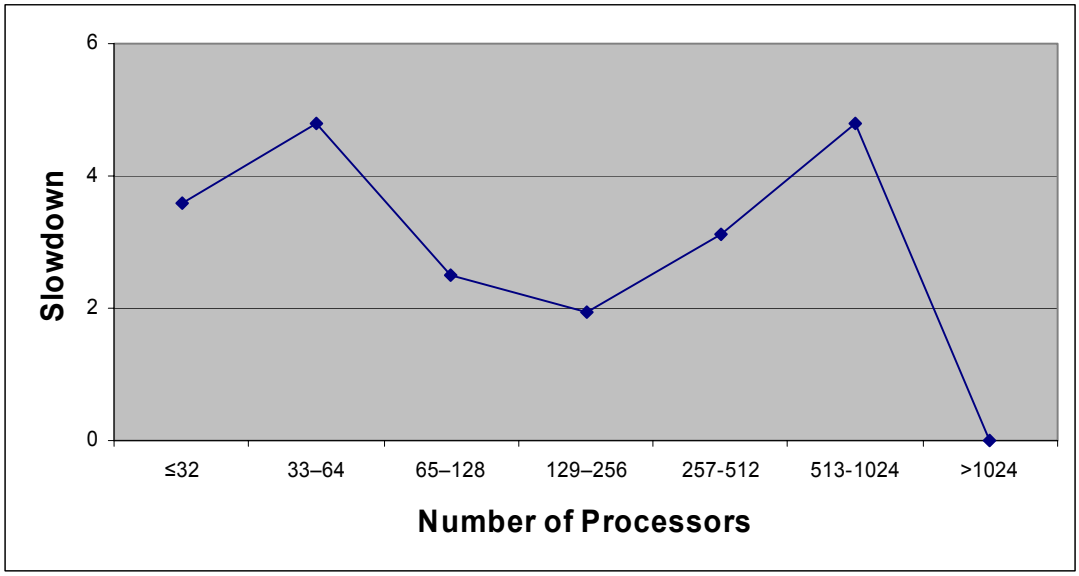
Slowdown is a widely used measure of the relative wait times of different classes of jobs. It is defined as:

Slowdown = (job run time + job wait time) / (job run time)

Slowdowns of less than around 10 are usually regarded as reasonable. The graph below plots slowdown against run-time (ignoring jobs of less than 5 minutes duration). Despite the good utilisation the pattern of slowdowns continues to be satisfactory.



In the graph below, we plot the slowdown figures against the number of processors used and ignoring the development jobs of less than 1 hour.

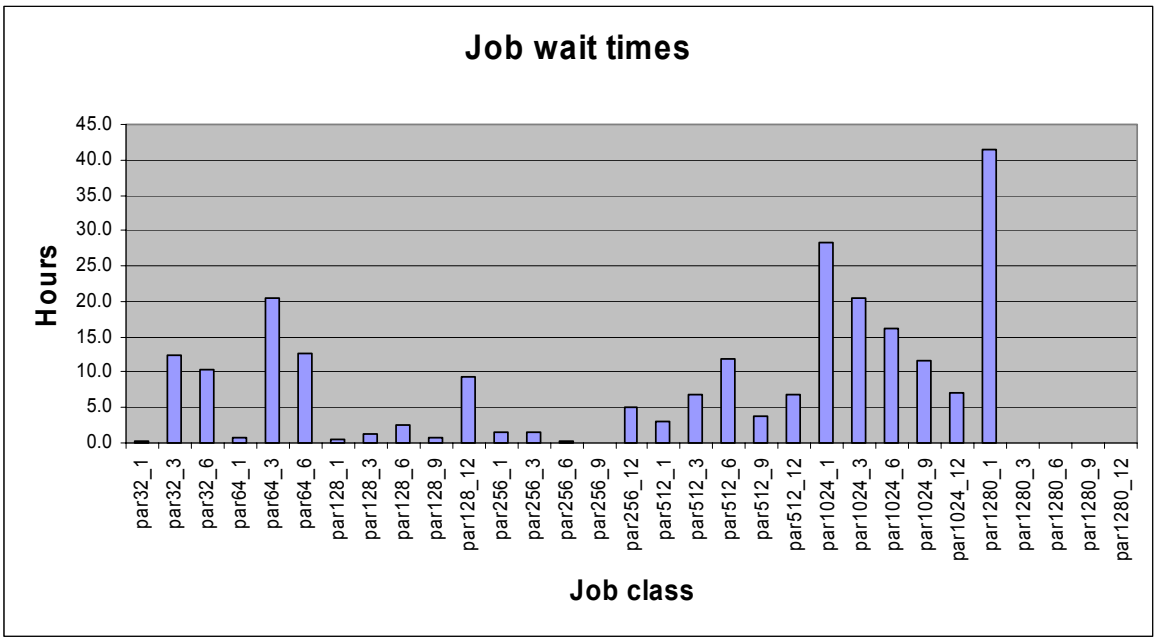


Job wait times

The following table and graph shows the average wait time (in hours) for each class of job. These are also satisfactory in general.

Job Class	*Category*	*Maximum Number of CPUs*	*Maximum Job length*	*Average wait time*	*Number of Jobs*
par32_1	parallel	32	1	0.3	2431
par32_3	parallel	32	3	12.3	82
par32_6	parallel	32	6	10.5	460
par64_1	parallel	64	1	0.8	371
par64_3	parallel	64	3	20.4	68
par64_6	parallel	64	6	12.6	335
par128_1	parallel	128	1	0.5	326
par128_3	parallel	128	3	1.3	43
par128_6	parallel	128	6	2.6	101
par128_9	parallel	128	9	0.7	1
par128_12	parallel	128	12	9.2	324
par256_1	parallel	256	1	1.4	241
par256_3	parallel	256	3	1.6	47
par256_6	parallel	256	6	0.4	22
par256_9	parallel	256	9	0.0	0
par256_12	parallel	256	12	5.1	45
par512_1	parallel	512	1	3.0	49
par512_3	parallel	512	3	6.9	13
par512_6	parallel	512	6	12.0	17
par512_9	parallel	512	9	3.8	4
par512_12	parallel	512	12	6.7	44

par1024_1	parallel	1024	1	28.4	13
par1024_3	parallel	1024	3	20.5	3
par1024_6	parallel	1024	6	16.1	11
par1024_9	parallel	1024	9	11.5	2
par1024_12	parallel	1024	12	7.0	21
par1280_1	parallel	1280	1	41.3	4
par1280_3	parallel	1280	3	0.0	0
par1280_6	parallel	1280	6	0.0	0
par1280_9	parallel	1280	9	0.0	0
par1280_12	parallel	1280	12	0.0	0
serial_1	serial	1	1	0.4	635
serial_12	serial	1	3	0.4	36
serial_3	serial	1	6	0.1	224
serial_6	serial	1	9	1.8	414
serial_9	serial	1	12	2.2	3
inter32_1	interactive	32	1	0.0	3619
course32_1	parallel	32	1	0.0	0



1.5 Disk Occupancy

Home Space

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

Consortium	*Disc Occupancy (Kb)*	*Disc Quota (Kb)*
b02	12,876,896	51,200,000
b03	4,384	51,200,000
b04	64	51,200,000
b05	16,802,368	51,200,000
b06	15,353,152	51,200,000
c01	82,284,928	102,400,000
e01	45,068,640	50,006,016
e02	23,280,416	39,760,896
e03	181,463,200	230,412,288
e04	95,840,480	102,400,000
e05	192,338,784	369,664,000
e06	240,414,272	307,200,000
e07	6,172,544	20,480,000
e08	16,058,176	20,480,000
e10	9,747,264	10,240,000
e11	38,168,768	102,400,000
e12	8,976,640	20,480,000
e14	53,980,576	102,400,000
e15	4,063,936	51,200,000
e16	47,392	20,480,000
e17	6,374,944	51,200,000
e18	30,677,088	40,960,000
e19	42,720	40,960,000
e20	43,079,712	61,440,000
e21	97,792	51,200,000
e22	96	10,240,000
e23	96	51,200,000
e24	686,656	51,200,000
e25	99,616	51,200,000
e26	16,577,248	20,480,000
e27	1,440	20,480,000
e28	128	40,960,000
e29	2,158,656	30,720,000
e30	64	40,960,000
e31	1,800,288	51,200,000
e32	96	51,200,000
n01	38,003,072	51,200,000
n02	95,759,168	110,592,000
n03	48,358,432	102,400,000
n04	131,581,472	307,198,976
n05	2,080	10,240,000
p01	34,133,152	40,960,000

x01	30,511,968	51,200,000
x02	8,956,000	20,480,000
z001	225,172,448	235,521,024
z002	42,528,896	49,153,024
z003	256	3,072
z004	72,766,848	102,400,000
z05	4,288,160	30,720,000
z06	48,863,776	51,200,000
z07	11,980,448	30,720,000
z09	3,296,992	51,200,000

Workspace

Consortium	*Disc Occupancy (Kb)*	*Disc Quota (Kb)*
b02	15,104	1,049,600
b03	19,367,360	102,400,000
b04	64	102,400,000
b05	6,372,000	102,400,000
b06	638,272	102,400,000
c01	61,285,024	102,400,000
e01	1,173,794,240	1,177,600,000
e02	8,291,328	10,240,000
e03	10,016	512,000,000
e04	1,573,478,688	2,252,800,000
e05	138,274,080	211,969,024
e06	253,213,568	409,600,000
e07	52,853,760	102,398,976
e08	139,232	1,024,000
e10	271,389,152	307,200,000
e11	192	102,400,000
e12	743,584	102,400,000
e14	74,058,432	102,400,000
e15	18,211,936	102,400,000
e16	192	61,440,000
e17	512	102,400,000
e18	160	81,920,000
e19	172,772,544	204,800,000
e20	466,532,960	1,024,000,000
e21	1,024	102,400,000
e22	96	20,480,000
e23	96	102,400,000
e24	101,929,408	102,400,000
e25	2,018,432	102,400,000
e26	128	40,960,000
e27	192	40,960,000
e28	6,014,240	81,920,000
e29	128	8,192,000
e30	64	81,920,000

e31	128	102,400,000
e32	96	102,400,000
n01	190,683,552	512,000,000
n02	1,224,508,480	1,504,257,024
n03	31,968	1,026,048
n04	325,977,056	768,000,000
n05	25,564,480	92,160,000
p01	1,022,464	1,024,000
x01	88,123,200	102,400,000
x02	128	20,480,000
z001	303,225,632	409,598,976
z002	296,448	788,480
z003	192	3,072
z004	24,885,312	25,600,000
z05	192	1,024,000
z06	26,024,256	102,400,000
z07	1,600	1,024
z09	53,248,352	102,400,000

1.6 Tape Archive

Consortium	*Usage (Tapes)*	*Quota (Tapes)*	*Files*	*Data (Gb)*
c01	2	2	8	16
e01	38	38	36748	3426
e03	5	5	18797	429
e04	4	14	1260	254
e26	2	2	72	11
n01	60	70	2394	5544
n02	50	50	72624	7079
n04	19	20	64038	2102
z001	2	2	4982	32
z002	3	4	1619	11
z06	1	3	833	68

Note that a tape is counted in the *Usage* column even if it is only partly occupied.

2 Support

2.1 Helpdesk

Classifications

Category	*Number*	*% of all*
Administrative	35	50.7
Technical	25	36.2
In-depth	9	13.0
PMR	0	0.0
TOTAL	69	100.0

The PMR category indicates in-depth queries that result in Problem Management Reports for IBM.

Service Area	*Number*	*% of all*
Phase 2 platform	61	88.4
Website	2	2.9
Other/general	6	8.7
TOTAL	69	100.0

Performance

All non-indepth queries	*Number*	*%*	*Target*
Finished within 24 Hours	53	88.3	75%
Finished within 72 Hours	60	100.0	97%
Finished after 72 Hours	0	0.0	

Administrative queries	*Number*	*%*	*Target*
Finished within 48 Hours	35	100.0	97%
Finished after 48 Hours	0	0.0	

Experts Handling Queries

Expert	*Admin*	*Technical*	*In-Depth*	*PMR*
epcc.ed.ac.uk	27	11	4	0
dl.ac.uk	0	3	3	0
Sysadm	7	11	2	0
Other people	1	0	0	0

2.2 Training

Title of Course	*Start Date*	*Length (Days)*	*Place days*	*HPCx User Days*	*HPCx Staff Days*
Introduction to High Performance Computing	22-Aug	1	25	16	7
Java for High Performance Computing	23-Aug	2	50	34	0
Practical Software Development	28-Aug	4	80	48	36

3 Staffing

3.1 Science Support Staffing

Daresbury Laboratory

Name	*Days*
Ashworth	8.1
Blake	1.2
Bush	22.0
Guest	5.5
Johnstone	10.5
Jones	3.8
Plummer	13.0
Sherwood	2.8
Sunderland	12.0
Thomas	5.0
Pickles	2.2
van Dam	1.0
Total (Days)	87.0
FTEs	4.9

EPCC

Name	*Days*
Simpson	7.9
Booth	17.1
Henty	13.2
Smith	17.6
Bull	10.5
Fisher	9.0
Hein	16.1
Jackson, A	3.4
Pringle	0.8
Reid	19.6
Murdoch	0.0
Carter	0.0
Breitmoser	0.0
Stratford	0.0
Nowell	0.7
Holden	11.5

Kartsaklis	12.2
Nazarova	0.7
Trew	5.8
Gray	8.9
D'Mellow	17.7
Helpdesk	4.3
Training	11.7
Total (Days)	188.5
FTEs	10.6

This month, we ran the Practical Software Development course which draws heavily on EPCC's industrial experiences. The course is therefore taught largely by staff who work on EPCC's commercial activities rather than by the HPCx team. This staff effort accounts for the 0.66 FTE labelled as 'Training', which includes the associated course organisation and updating in addition to delivery

Overall Levels

	FTEs
DL	4.9
EPCC	10.6
Total	15.5

3.2 Systems Staffing

Name	*Days*
Andrews	12.8
Blake	0.0
Brown	23.0
Fisher	9.5
Georgeson	15.8
Franks	11.3
Jones	0.0
Shore	12.8
BITD	22.0
Total (days)	107.0
FTEs	6.0

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.

4 Summary of Performance Metrics

Metric	*TSL*	*FSL*	*Monthly Measurement*
Technology serviceability	80%	99.2%	100.0%
Technology MTBF (hours)	200	300	∞
Number of AV FTEs	7.5	10	14.9
Number of training days per month	22.5/12	30/12	20/8
Non in-depth queries resolved within 3 days	85%	97%	100.0%
Number of A&M FTEs	3.75	5.75	5.4
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

Code	*Class*	*Title*	*PI*
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 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

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 H. 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
z09		HECToR Benchmarking	Dr Edward Smyth

PPARC Projects

Code	*Class*	*Title*	*PI*
p01	1	Atomic Physics and Astrophysics	Prof Alan Hibbert

NERC Projects

Code	*Class*	*Title*	*PI*
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

Code	*Class*	*Title*	*PI*
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

CCLRC Projects

Code	*Class*	*Title*	*PI*
c01	1	Daresbury Laboratory Facilities Agreement Consortium	Dr Richard J Blake

Externally-funded Projects

Code	*Title*	*PI*
x01	HPC-Europa	Dr J-C Desplat
x02	OHM Ltd	Mr Mark Westwood

HPCx Projects

Code	*Title*	*PI*
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

Code	*Class*	*Title*	*PI*
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