

CSAR Service - Management Report

September 2001

This report documents the quality of the CSAR service during the month of September 2001.

A more comprehensive report is provided quarterly, which additionally covers wider aspects of the Service such as information on Training, Application Support and Value-Added services.

This and other such reports are made available through the Web to staff within EPSRC and the other Research Councils, to CfS staff and CSAR Service users. The reports are indexed in a similar way to that which other useful information and news are listed for selection.

1. Introduction

This document gives information on Service Quality and on actual usage of the CSAR Service during the reporting period of September 2001. The information, in particular, covers the availability and usage of the following three main CSAR Service High Performance Computing (HPC) systems:

- Cray T3E-1200E/776 (Turing)
- SGI Origin2000/128 (Fermat)
- SGI Origin3000/512 (Green)

The information is provided in both textual and graphical form, so that it is easier to see trends and variances.

September has seen the workload of the three primary systems remaining high.

The percentage of Turing CPU capacity used by jobs larger than 64 PEs was 72%.

September also saw the utilisation on the Origin 3000 (Green) climbing, and the percentage of Green CPU capacity used by jobs larger than 64 PEs was 61%.

2. Service Quality

This section covers overall Customer Performance Assessment Ratings (CPARS), HPC System availability and usage, Service Quality Tokens and other information concerning issues, progress and plans for the CSAR Service.

2.1 CPARS

Table 1 gives the measure by which the quality of the CSAR Service is judged. It identifies the metrics and performance targets, with colour coding so that different levels of achievement against targets can be readily identified. Unsatisfactory actual performance will trigger corrective action.

CSAR Service - Service Quality Report - Performance Targets

Service Quality Measure	Performance Targets					
	White	Blue	Green	Yellow	Orange	Red
HPC Services Availability						
Availability in Core Time (% of time)	> 99.9%	> 99.5%	> 99.2%	> 98.5%	> 95%	95% or less
Availability out of Core Time (% of time)	> 99.8%	> 99.5%	> 99.2%	> 98.5%	> 95%	95% or less
Number of Failures in month	0	1	2 to 3	4	5	> 5
Mean Time between failures in 52 week rolling period (hours)	>750	>500	>300	>200	>150	otherwise
Fujitsu Service Availability						
Availability in Core Time (% of time)	> 99.9%	> 99.5%	> 99.2%	> 98.5%	> 95%	95% or less
Availability out of Core Time (% of time)	> 99.8%	> 99.5%	> 99.2%	> 98.5%	> 95%	95% or less
Help Desk						
Non In-depth Queries - Max Time to resolve 50% of all queries	< 1/4	< 1/2	< 1	< 2	< 4	4 or more
Non In-depth Queries - Max Time to resolve 95% of all queries	< 1/2	< 1	< 2	< 3	< 5	5 or more
Administrative Queries - Max Time to resolve 95% of all queries	< 1/2	< 1	< 2	< 3	< 5	5 or more
Help Desk Telephone - % of calls answered within 2 minutes	>98%	> 95%	> 90%	> 85%	> 80%	80% or less
Others						
Normal Media Exchange Requests - average response time	< 1/2	< 1	< 2	< 3	< 5	5 or more
New User Registration Time (working days)	< 1/2	< 1	< 2	< 3	< 4	otherwise
Management Report Delivery Times (working days)	< 1	< 5	< 10	< 12	< 15	otherwise
System Maintenance - no. of sessions taken per system in the month	0	1	2	3	4	otherwise

Table 1

Table 2 gives actual performance information for the period of September 1st to 30th inclusive. Overall, the CPARS Performance Achievement in September was satisfactory (see Table 3); i.e. Green measured against the CPARS performance targets. The Fujitsu availability figures are included in Table 2, but not Table 3 as they have zero weighting in CPARS terms.

CSAR Service - Service Quality Report - Actual Performance Achievement

Service Quality Measure	2000/1											
	Oct	Nov	Dec	Jan	Feb	March	April	May	June	July	Aug	Sept
HPC Services Availability												
Availability in Core Time (% of time)	100%	100%	94.90%	99.70%	99.70%	100%	100%	99.70%	99.70%	98.49%	98.49%	98.49%
Availability out of Core Time (% of time)	100%	99.40	98.49%	99.50%	99.40	99.40	99.40	99.40	99.40	98.49%	100%	99.40
Number of Failures in month	0	2	4	1	1	1	1	3	3	4	2	2
Mean Time between failures in 52 week rolling period (hours)	1095	673	584	584	626	674	674	584	584	438	398	365
Fujitsu Service Availability												
Availability in Core Time (% of time)	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Availability out of Core Time (% of time)	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Help Desk												
Non In-depth Queries - Max Time to resolve 50% of all queries	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25	<0.25
Non In-depth Queries - Max Time to resolve 95% of all queries	<1	<3	<3	<5	<5	<3	<5	<2	<2	<1	<1	<1
Administrative Queries - Max Time to resolve 95% of all queries	<0.5	<0.5	<5	<2	<2	<3	<0.5	<0.5	<0.5	<1	<2	<1
Help Desk Telephone - % of calls answered within 2 minutes	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Others												
Normal Media Exchange Requests - average response time	0	<0.5	<0.5	<0.5	<0.5	0	0	<0.5	<0.5	<0.5	<0.5	<0.5
New User Registration Time (working days)	0	0	0	0	0	0	0	0	0	0	0	0
Management Report Delivery Times (working days)	10	10	10	10	10	10	12	10	10	10	10	10
System Maintenance - no. of sessions taken per system in the month	1	2	1	0	2	1	2	0	0	1	2	2

Table 2

Notes:

- HPC Services Availability has been calculated using the following formulae, based on the relative NPB performance of Turing and Fermat at installation:

$$[\text{Turing availability} \times 122 / (122 + 3.5)] + [\text{Fermat availability} \times 3.5 / (122 + 3.5) \times 1.556]$$
- Mean Time between failures for Service Credits is formally calculated based on a rolling 12 month period.

Table 3 gives Service Credit values for the month of September. These will be accounted on a quarterly basis, formally from the Go-Live Date. The values are calculated according to agreed Service Credit Ratings and Weightings.

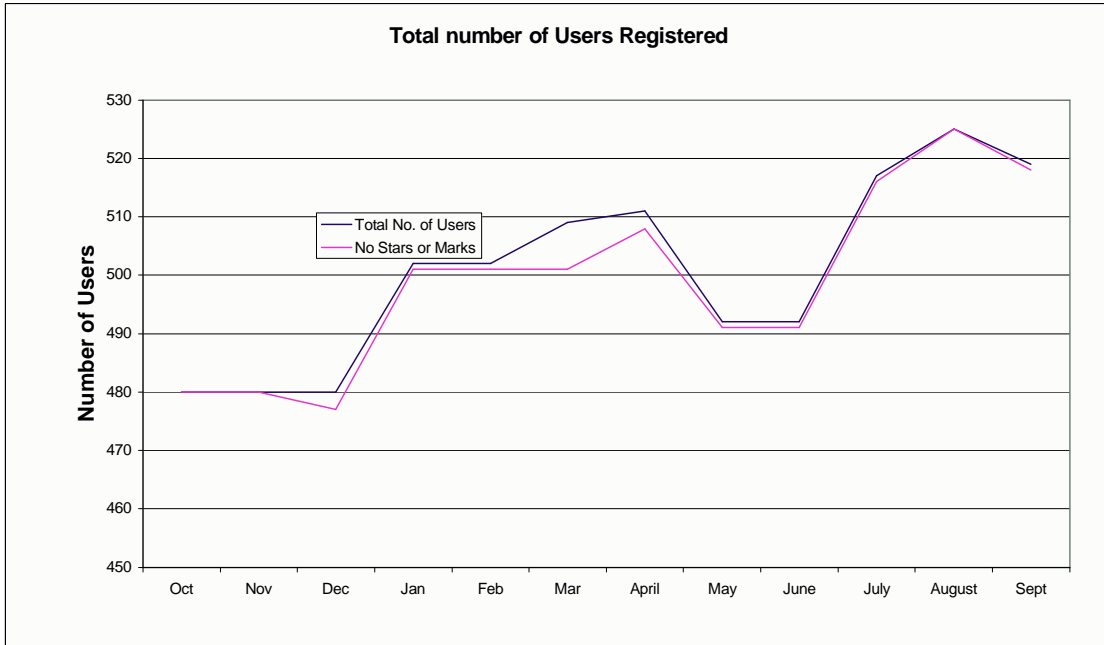
CSAR Service - Service Quality Report - Service Credits

Service Quality Measure	2000/1											
	Oct	Nov	Dec	Jan	Feb	March	April	May	June	July	Aug	Sept
HPC Services Availability												
Availability in Core Time (% of time)	-0.058	-0.058	0.195	-0.039	-0.039	-0.058	-0.058	-0.039	-0.039	0.039	0.039	0.039
Availability out of Core Time (% of time)	-0.047	0	0.039	-0.039	0	0	0	0	0	0.039	-0.047	0
Number of Failures in month	-0.009	0	0.008	-0.008	-0.008	-0.008	-0.008	0	0	0.008	0	0
Mean Time between failures in 52 week rolling period (hours)	-0.009	-0.008	-0.008	-0.008	-0.008	-0.008	-0.008	-0.008	-0.008	0	0	0
Help Desk												
Non In-depth Queries - Max Time to resolve 50% of all queries	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019
Non In-depth Queries - Max Time to resolve 95% of all queries	-0.016	-0.016	0.016	0.016	0.031	0.031	0.016	0	0	0.000	-0.016	0.000
Administrative Queries - Max Time to resolve 95% of all queries	-0.019	-0.019	0.046	0	0	0.016	-0.019	-0.019	-0.019	-0.016	0.016	0.000
Help Desk Telephone - % of calls answered within 2 minutes	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004	-0.004
Others												
Normal Media Exchange Requests - average response time	0	-0.002	-0.002	-0.002	-0.002	0	0	-0.002	-0.002	-0.002	0	-0.002
New User Registration Time (working days)	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019	-0.019
Management Report Delivery Times (working days)	0	0	0	0	0	0	0.003	0	0	0	0	0
System Maintenance - no. of sessions taken per system in the month	-0.003	0	-0.003	-0.004	0	-0.003	-0.003	-0.004	-0.004	-0.003	0	0
Monthly Total & overall Service Quality Rating for each period:	-0.10	-0.07	0.12	-0.06	-0.03	-0.04	-0.06	-0.06	-0.06	0.01	-0.02	0.00

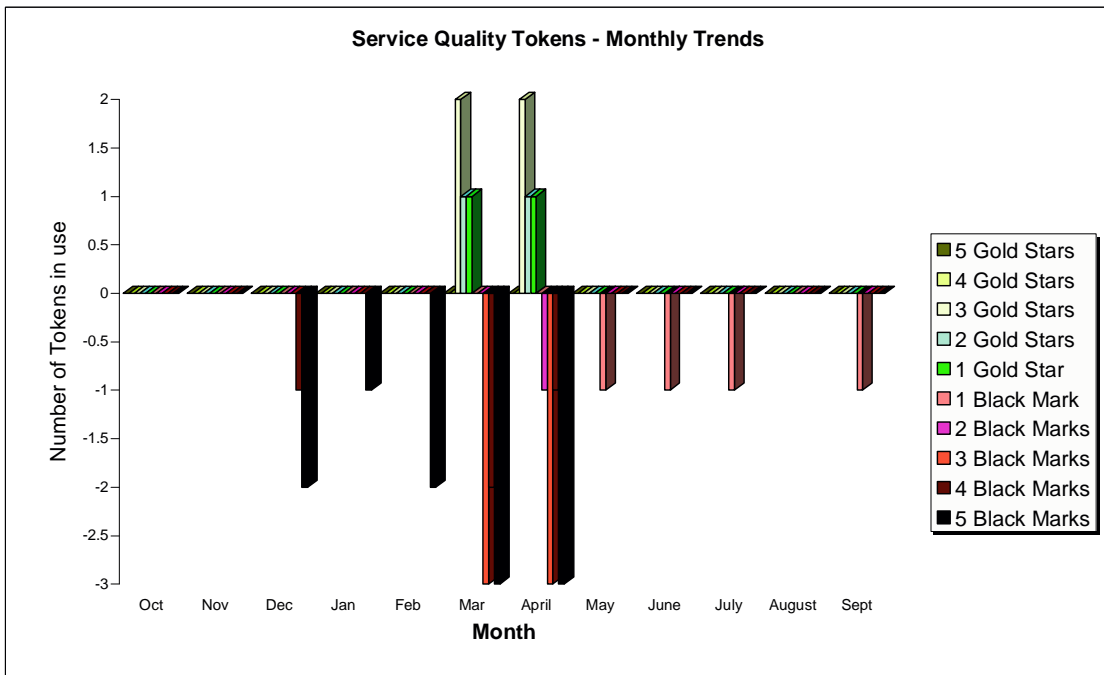
Table 3

2.2 Service Quality Tokens

The current position at the end of September 2001 is that one of the 519 registered users of the CSAR Service had registered a black mark against the service.



The graph above shows the total number of registered users on the CSAR Service and the number of users holding a neutral view of the service.



The graph below illustrates the monthly usage trend of quality tokens:

The current status of the Stendahl tokens is that one user has allocated a black marks against the system for login problems.

SUMMARY OF SERVICE QUALITY TOKEN USAGE

No of Stars or Marks	Consortia	Date Allocated	Reason Given
1 Black Mark	cse006	25/09/01	Login problems continuing

2.3 Throughput Target against Baseline

The Baseline Target for throughput was fully achieved this month due to plenty of work over the period. The actual usage figure was 148% of Baseline capacity.

Job Throughput Against Baseline CSAR Service Provision

Period: 1st to 30th September 2001

	Baseline Capacity for Period (T3E PE Hours)	Actual Usage in Period (T3E PE Hours)	Actual % Utilisation c/w Baseline during Period
1. Has CfS failed to deliver Baseline MPP Computing Capacity for EPSRC?	347,855	515,015	148.05%
2. Have Users submitted work demanding > 110% of the Baseline during period?	347,855	527,403	Yes
3. Are there User Jobs outstanding at the end of the period over 4 days old?		Number of Jobs at least 4 days old at end Period 3	Number of Jobs at least 4 days old at end Period is not zero (Yes/No)? Yes
4. Have Users submitted work demands above 90% of the Baseline during period?		Minimum Job Time Demands as % of Baseline during Period 89%	Minimum Job Time Demand above 90% of Baseline during Period (Yes/No)? Yes
5. Majority of Job Queues contained jobs from Users for more than 97% during period?	Number of standard Job Queues (ignoring priorities) 4	Average % of time each queue contained jobs in the Period 63.0%	Average % of time each queue contained jobs in the Period is > 97%? No

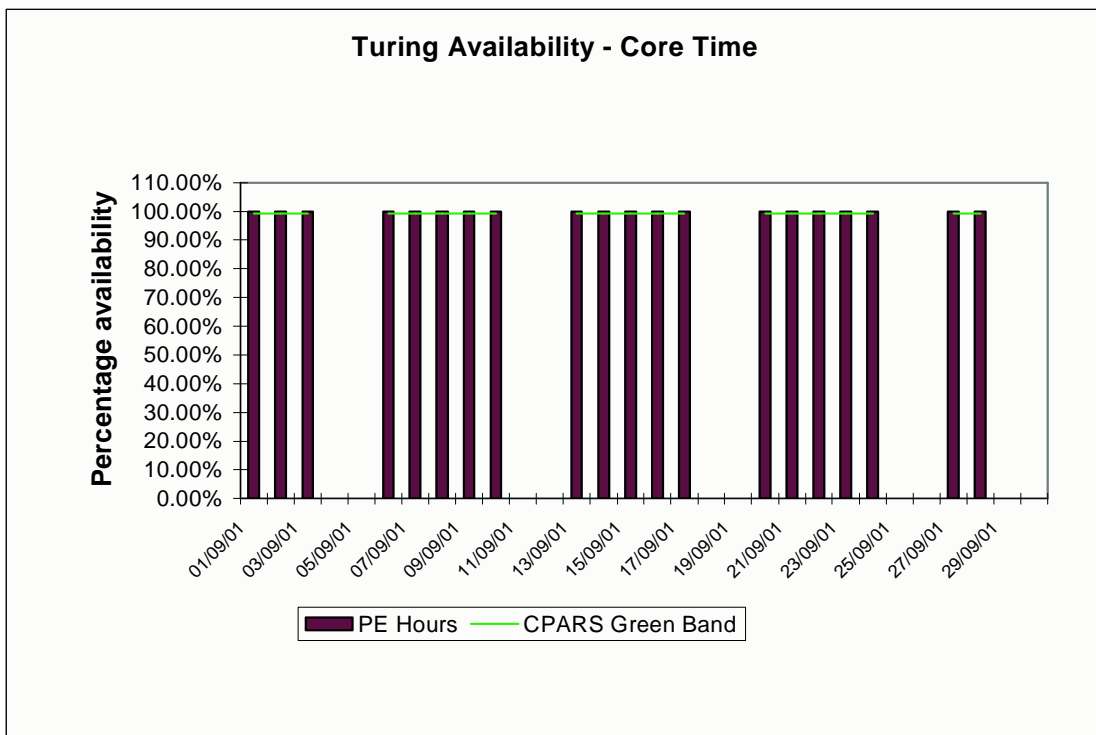
3. System Availability

Service availability each reporting period is calculated as a percentage of actual availability time over theoretical maximum time, after accounting for planned breaks in service for preventative maintenance.

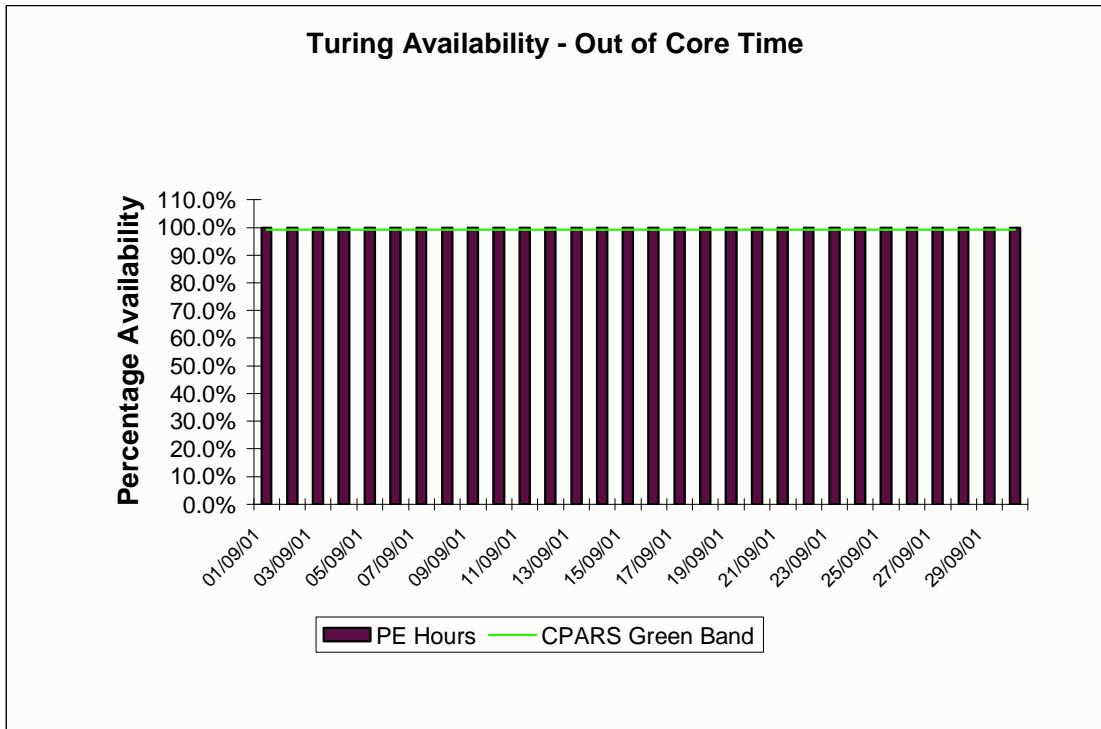
3.1 Cray T3E-1200E System (Turing)

The following graphs show the availability of Turing both in core time and out of core time respectively during the period of 1st to 30th September.

Turing availability for September:



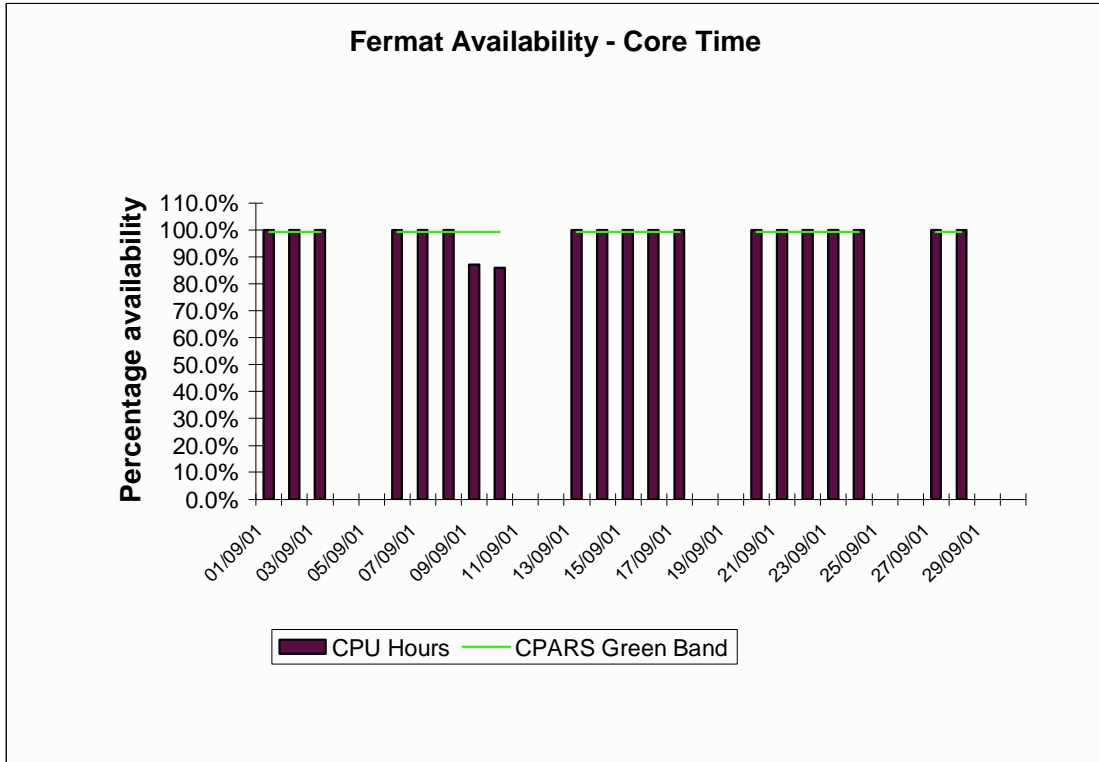
Availability of Turing in core time during September was excellent.



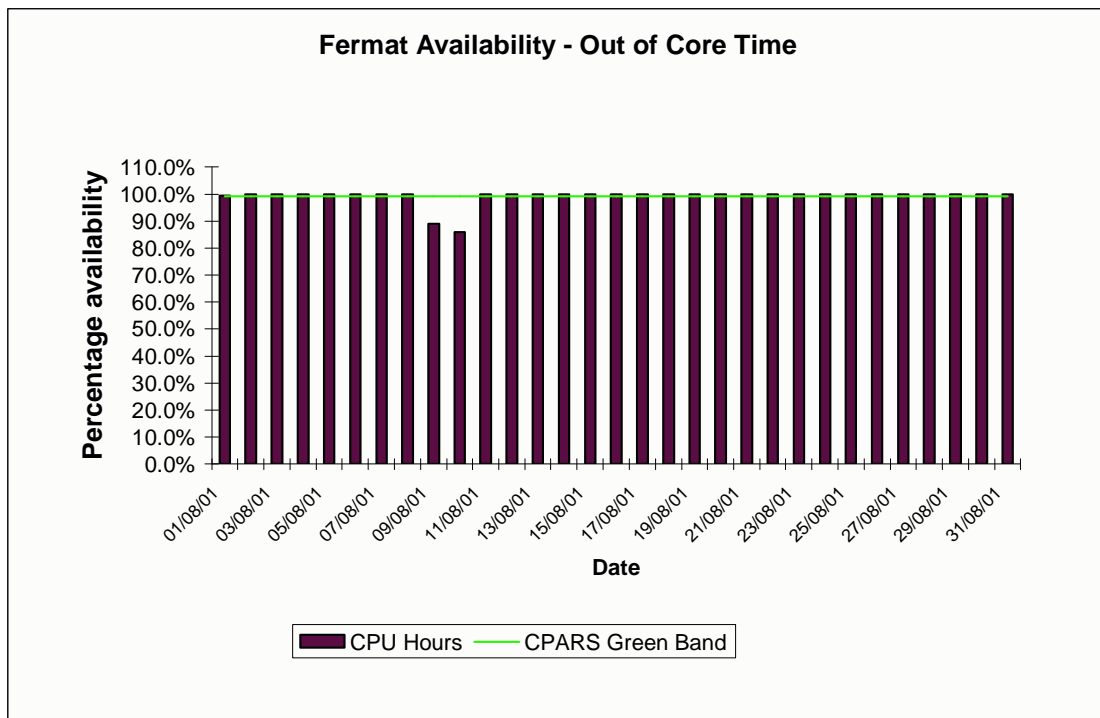
Availability of Turing out of core time during September was excellent.

3.2 SGI Origin2000 System (Fermat)

The following graphs show the availability of Fermat both in core time and out of core time respectively.



Availability of Fermat in core time during September was good with the exception of periods of unscheduled downtime on both the 9th & 10th of the month.



Availability of Fermat out of core time during September was good with the exception of the 9th & 10th of the month.

4. HPC Services Usage

Usage information is given in tabular form, in Appendices, and in graphical format. The system usage information for the period of September 1st to 30th, is provided by Project/User Group, totalled by Research Council and overall. This covers:

- CPU usage Turing: 515,015 PE Hours Fermat (Batch): 34,106 Hours
- Fermat (Interactive): 1,810 CPU Hours
- Green: 169,704 Hours
- Fujitsu CPU usage Fuji: 2,230 CPU Hours
- User Disk allocation Turing: 73.14 GB Years Fermat: 69.11 GB Years
- HSM/tape usage 1,343.61 GB Years

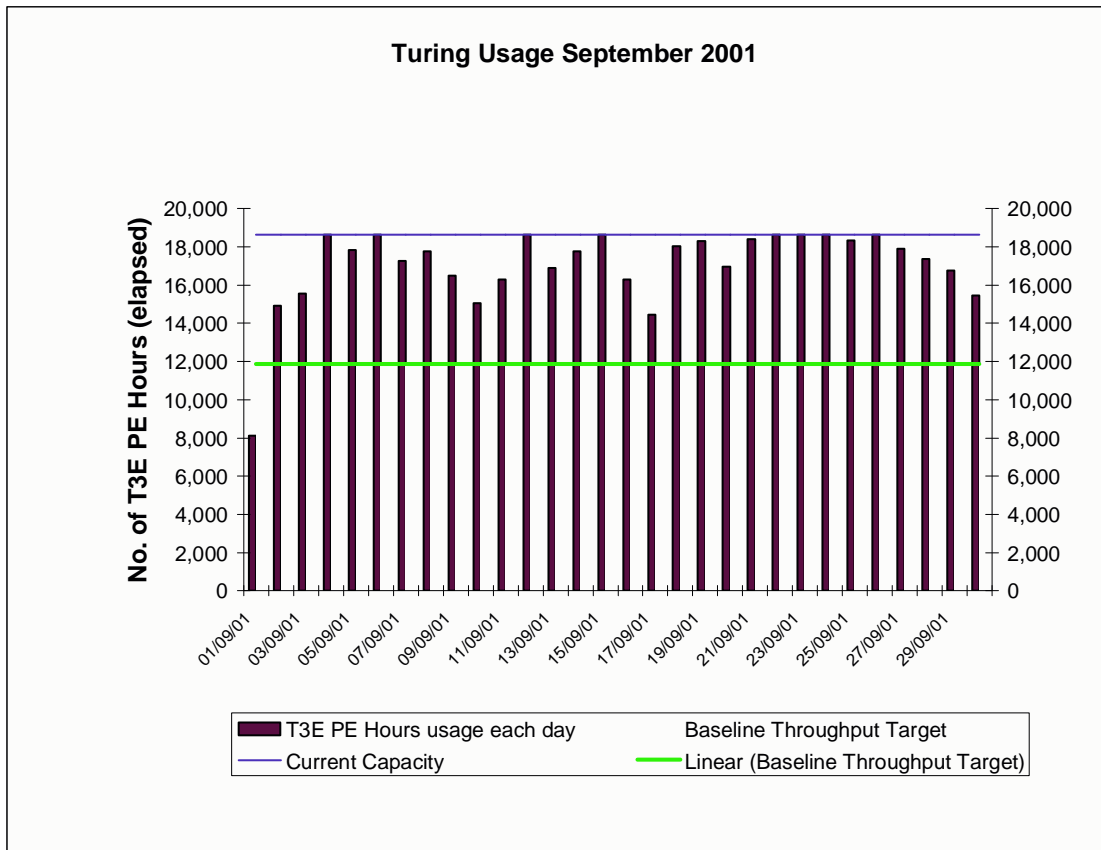
In addition, the following graphs are provided to illustrate usage per month, historically:

- a) MPP (T3E/Origin) Usage by month, showing usage each month of CPU (MFOP Years as per NPB), split by Research Council and by system. The Baseline and the overall Capacity are shown by overlaid horizontal lines.
- b) SMP (Origin) Usage by month, showing usage each month in CPU Hours, split by Research Council and giving the equivalent GFLOP-Years as per NPB. The Baseline Capacity is shown by an overlaid horizontal line.
- c) High Performance Disk (T3E) allocated for User Data by month, showing the allocated space each month in GBytes, split by Research Council. The Baseline Capacity (1 Terabyte) is shown by an overlaid horizontal line.
- d) Medium Performance Disk (Origin) allocated for User Data by month, showing the allocated space each month in GBytes, split by Research Council. The Baseline Capacity (1.5 Terabytes) is shown by an overlaid horizontal line.
- e) HSM/Tape Usage (T3E) by month, showing the volumes held each in GBytes, split by Research Council. The Baseline Capacity (16 Terabytes) available will be shown by an overlaid horizontal line.

4.1 Cray T3E-1200E System (Turing)

The following graph shows the usage of Turing during each day of September 2001. Note that there is some variance on a day-to-day basis as the accounts record job times, and thus CPU usage figures, at the time of job completion which could be the second actual day for large jobs. At present, there is a 24 hour limit on jobs so that they are check-pointed, and computational time lost due to any failure is well managed. Higher limits can be set for individual jobs on request.

Turing usage for September:



The above usage graph for the Turing system shows that the overall workload was variable.

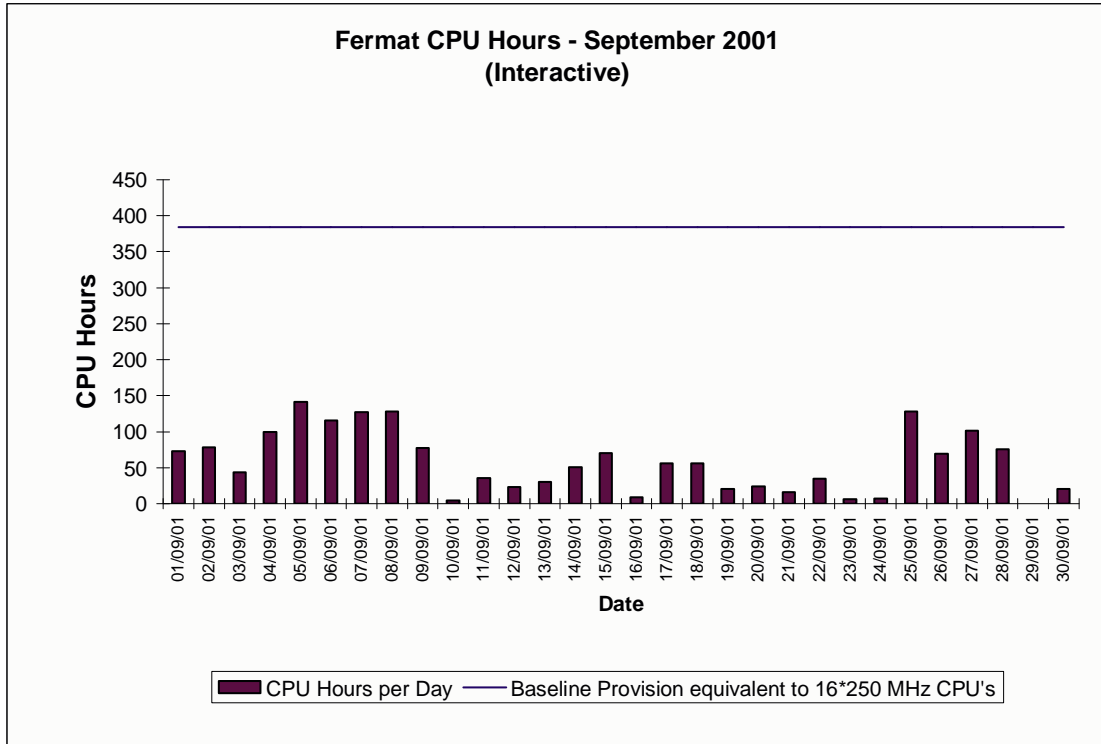
The graph also indicates the workload reached 100% of maximum theoretical capacity some part of the month.

Fine tuning of the CfS scheduling system will continue to ensure minimal wasting of PE resource, in order to fit in a number of different sized jobs (e.g. 32, 64, 128, 256) thus facilitating maximised job throughput.

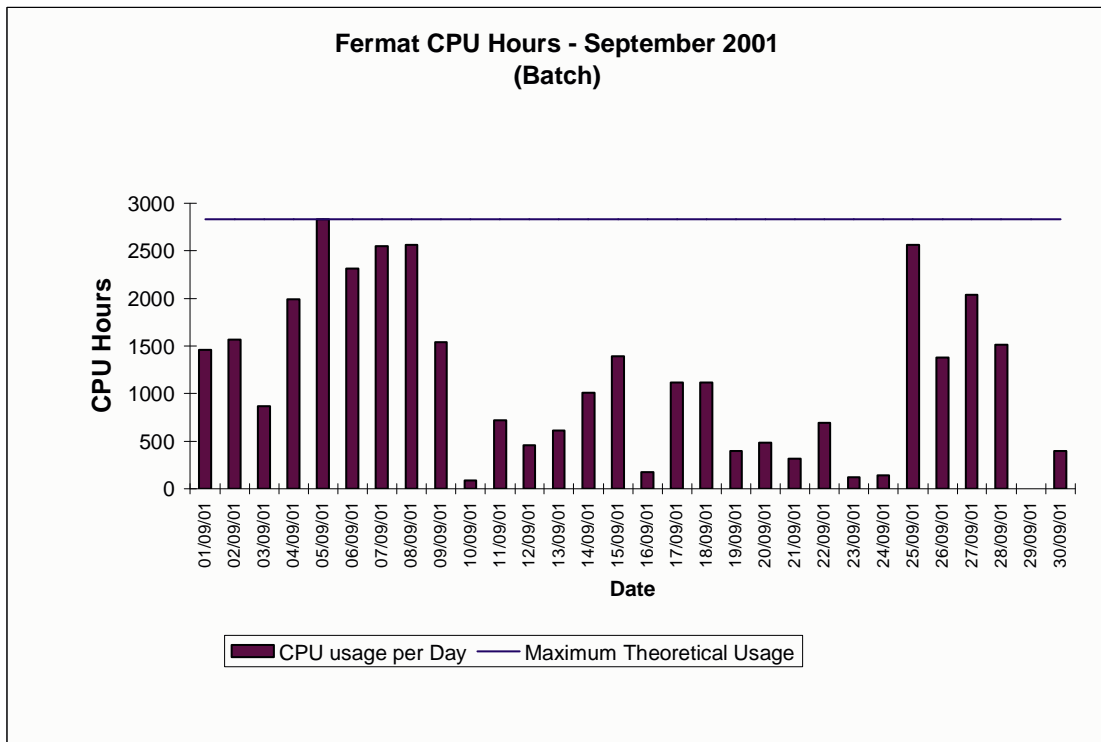
In particular, Turing will continue to start large jobs above 256 PEs, including 512 PEs, when they are queued subject to the overall workload.

4.2 SGI Origin2000 System (Fermat)

The usage of the Origin system was low. The groups most heavily using the Fermat system are CSE006 (Briddon), CSN006 (Price), CSN015 (Proctor) and HPCI Daresbury.

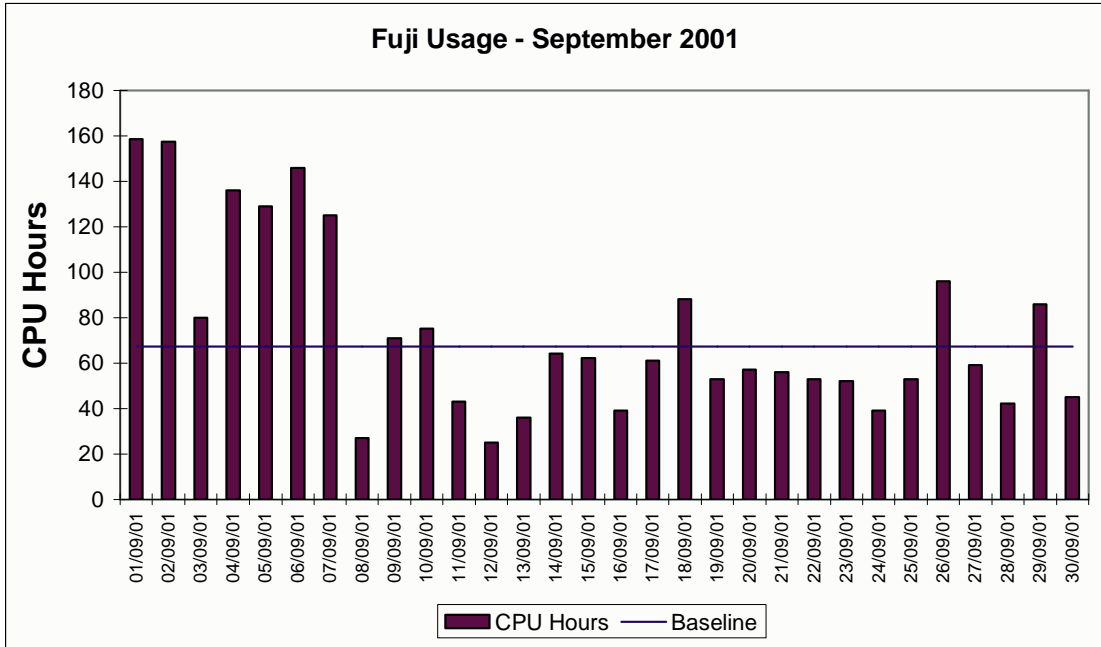


The graph above shows the interactive usage of the upgraded Origin 2000 (Fermat).



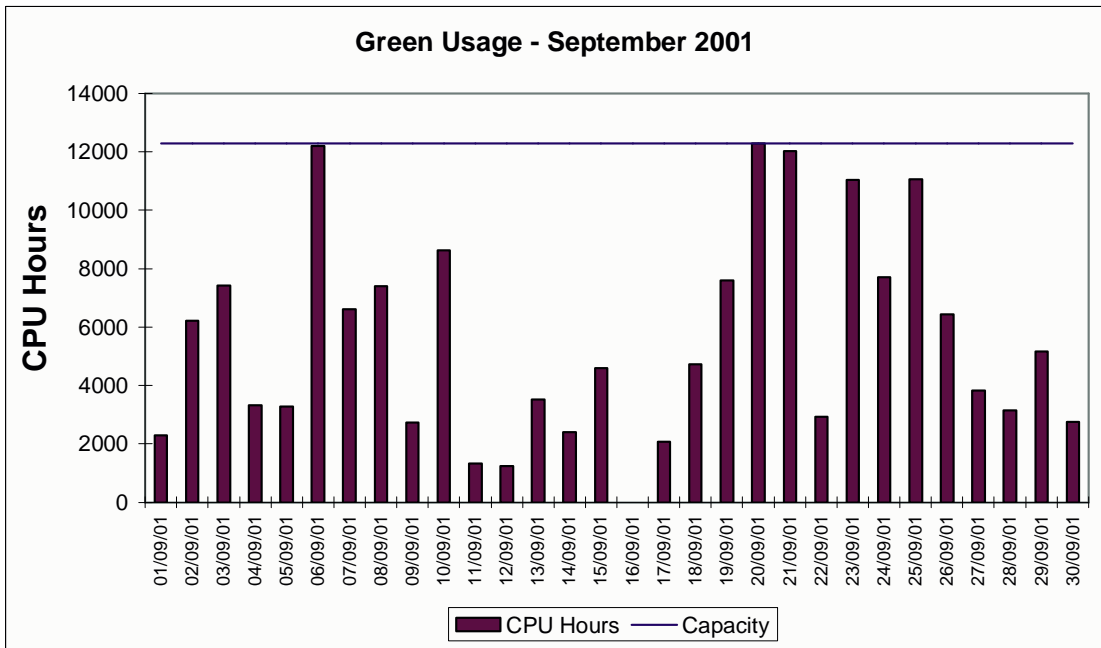
The above graph to a different scale shows the variable batch utilisation of the Origin 128.

4.3 Fujitsu VPP 300/8 System (Fuji)



Fuji utilisation was again variable over the month with the overall position resulting in usage above baseline.

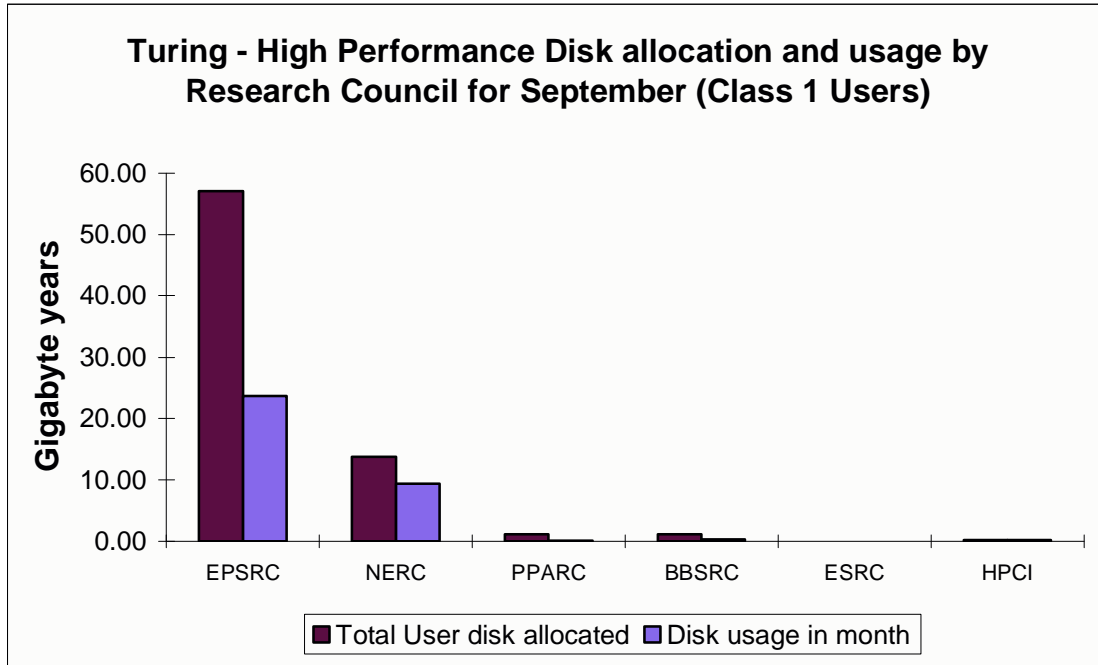
4.4 SGI Origin3000 System (Green)



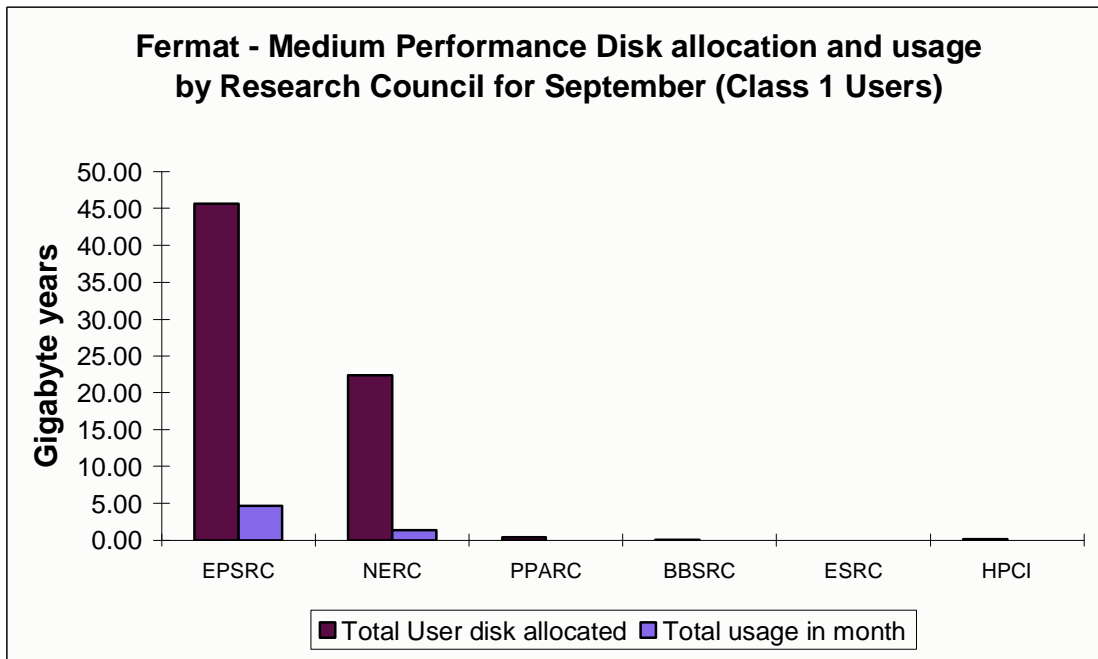
The above graph shows the utilisation of the now upgraded Green for the month of September, which saw the system running at 45% of capacity on average.

4.5 Disk/HSM Usage Charts

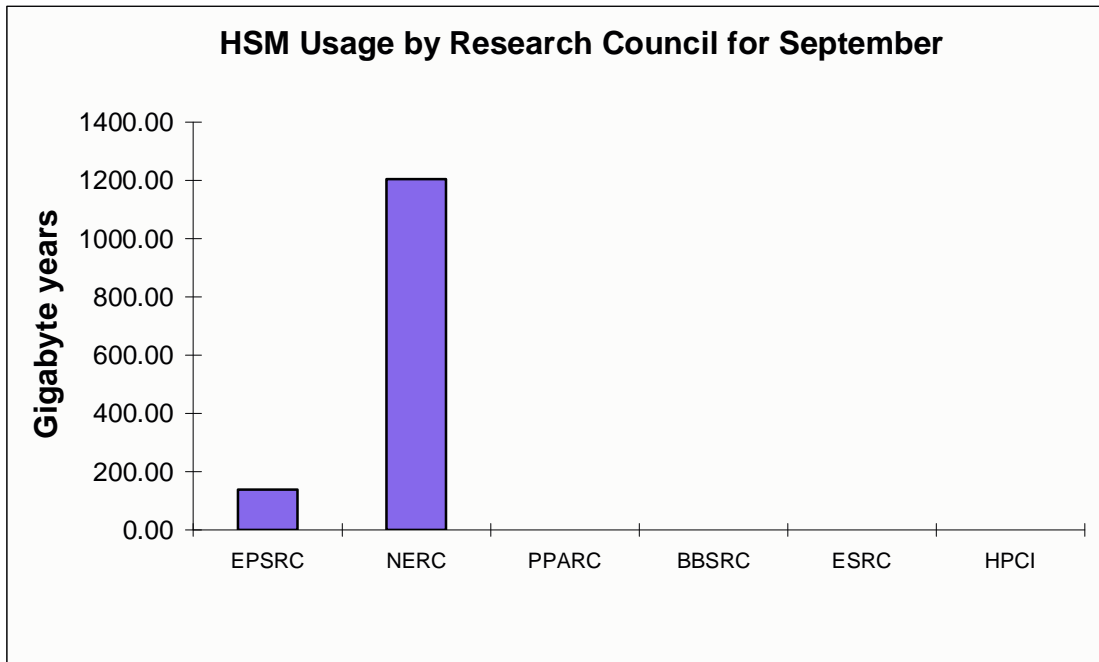
The graphs below show current disk and HSM allocations and usage.



The preceding graph shows actual usage on average against the current allocation of disk on the Turing system.

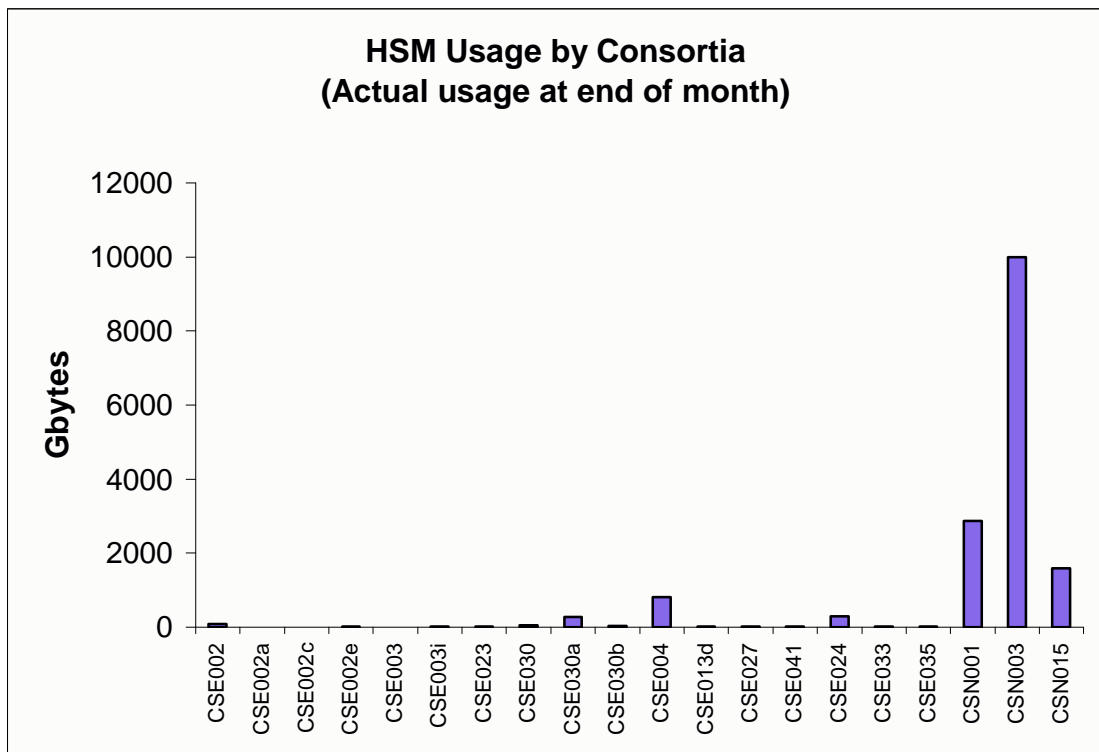


The above graph shows the disk allocations against usage on average of the disk on Fermat.

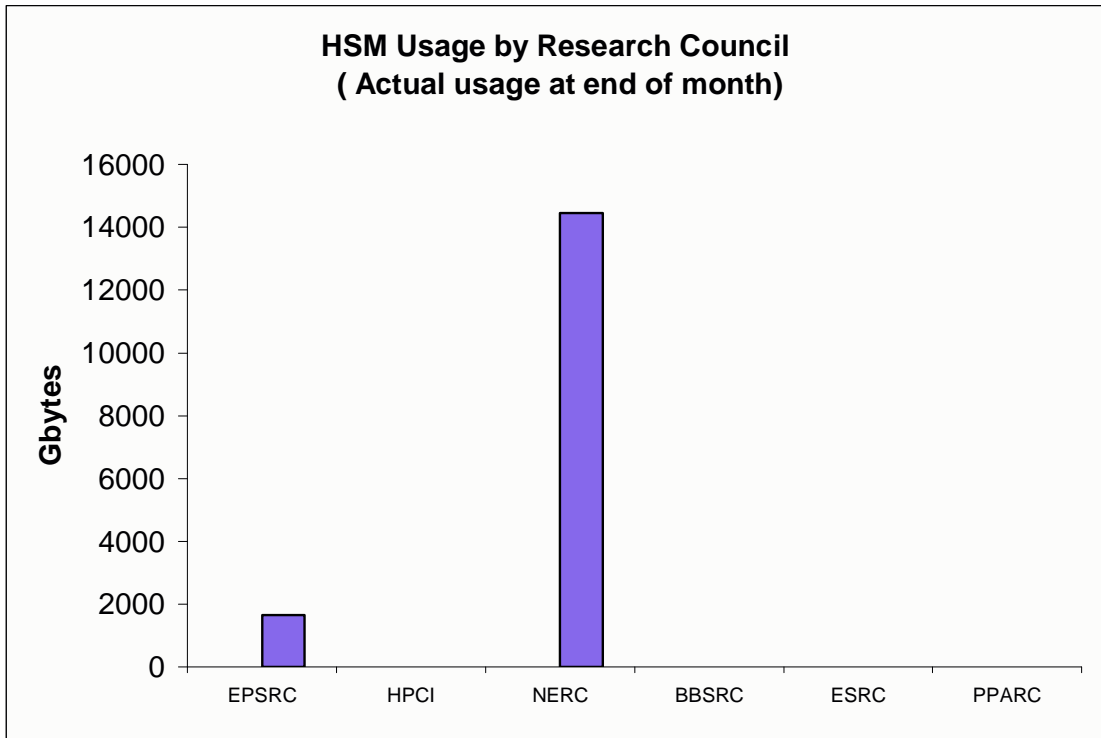


The above graph shows the total usage of the HSM facility by Research Council.

The next two graphs give actual usage of HSM by Consortia and by Research Council.

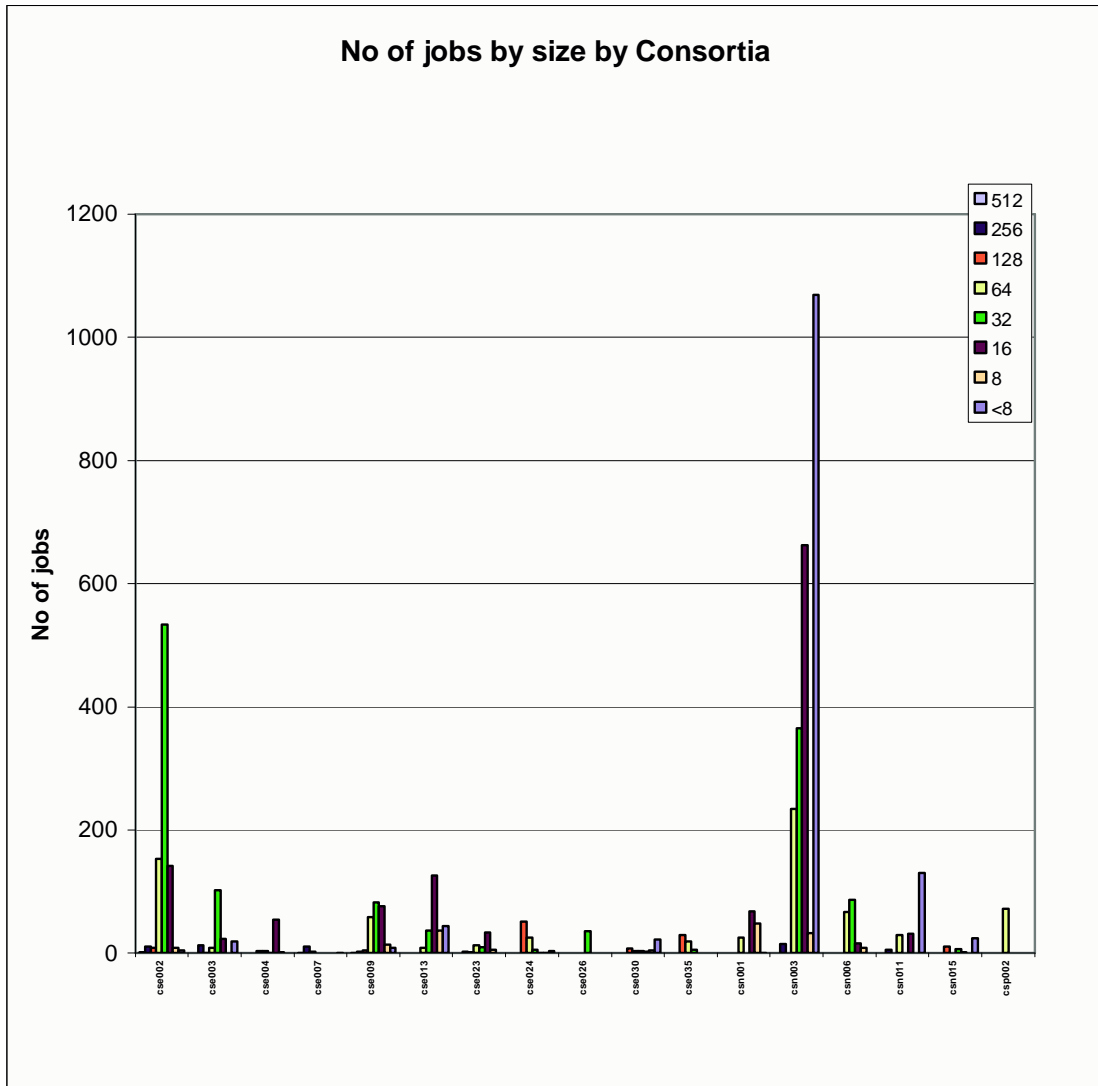


CSE002 (Gillan), CSE003 (Taylor) CSE004 (Sandham), CSE024 (Tennyson), CSN001 (Webb), CSN003 (O'Neill) & CSN015 (Proctor) were the major users of HSM resource.



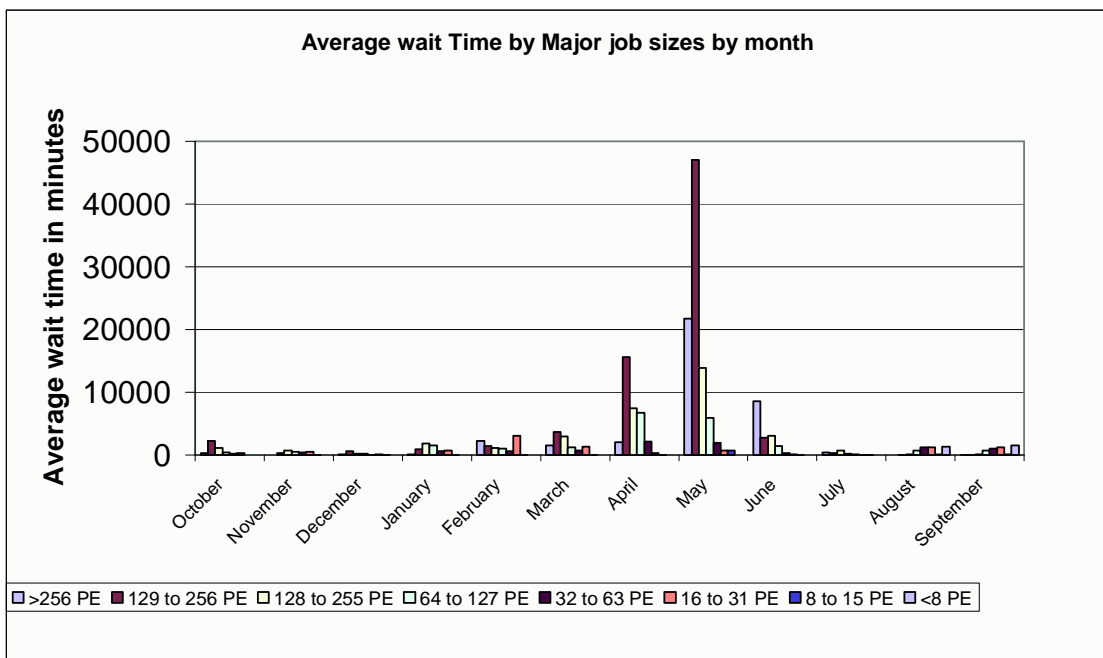
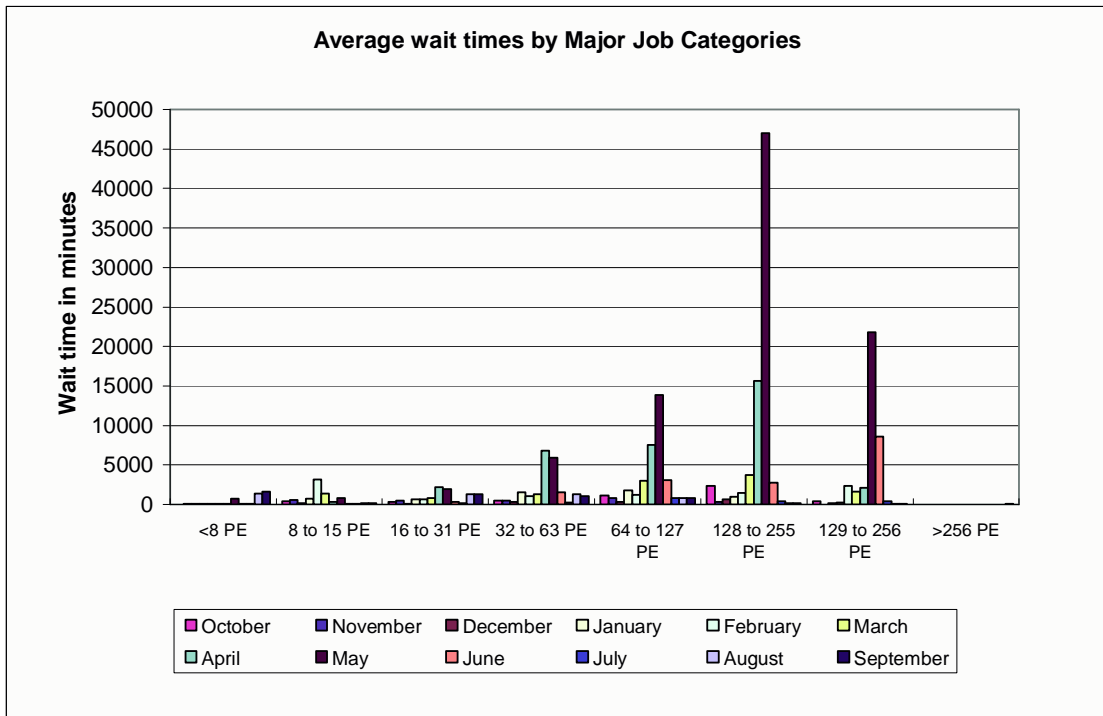
4.6 Processor Usage and Job Statistics Charts

Job statistics for Turing:

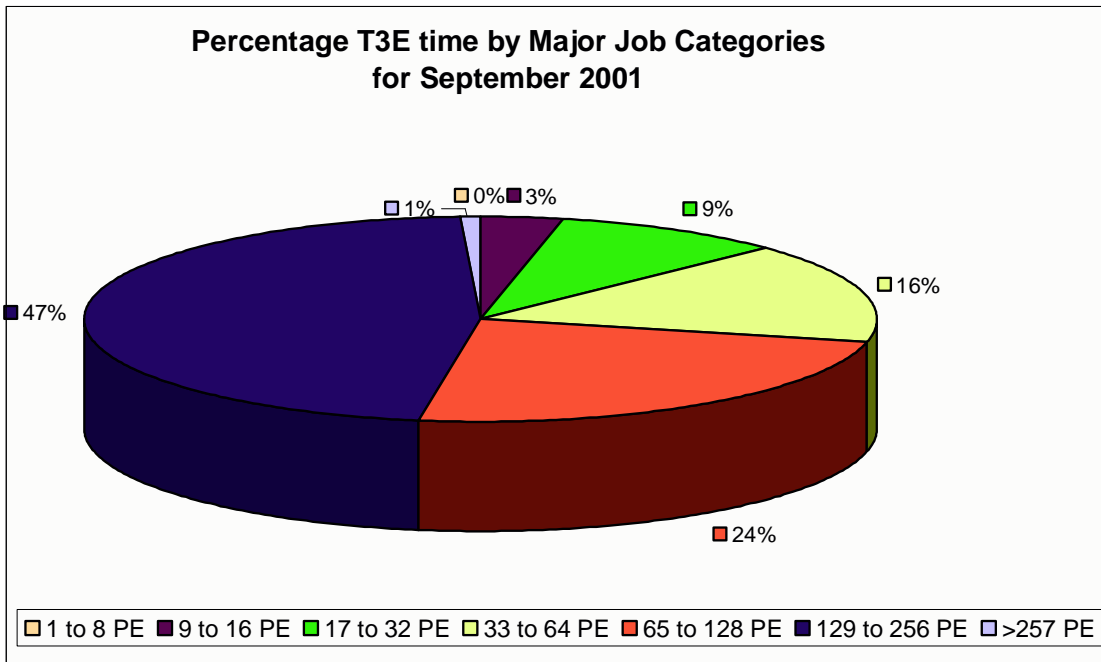


The above graph shows the number of jobs of the major sizes run in the period 1st to 30th September 2001.

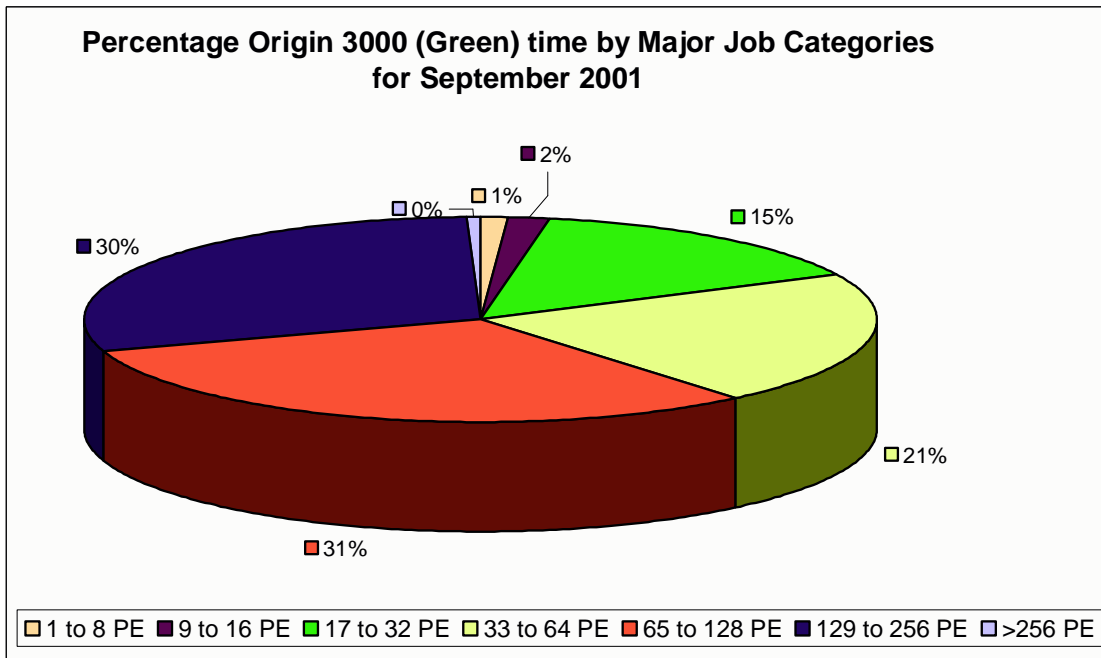
The next graph shows the wait times in minutes on Turing for the major categories of jobs.



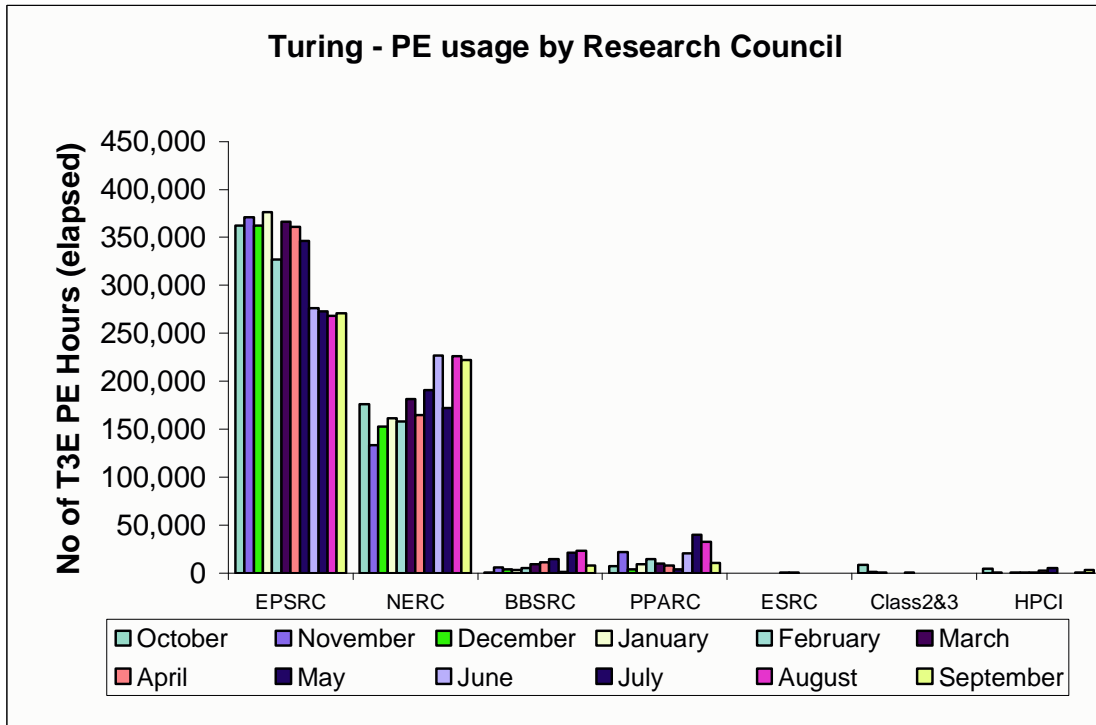
The chart above shows the average wait time trend on Turing over the last 12 months. Wait times for all jobs have fallen as Green is now in full production usage as a 512 PE machine. The trend of falling job times has levelled off over the past two months.



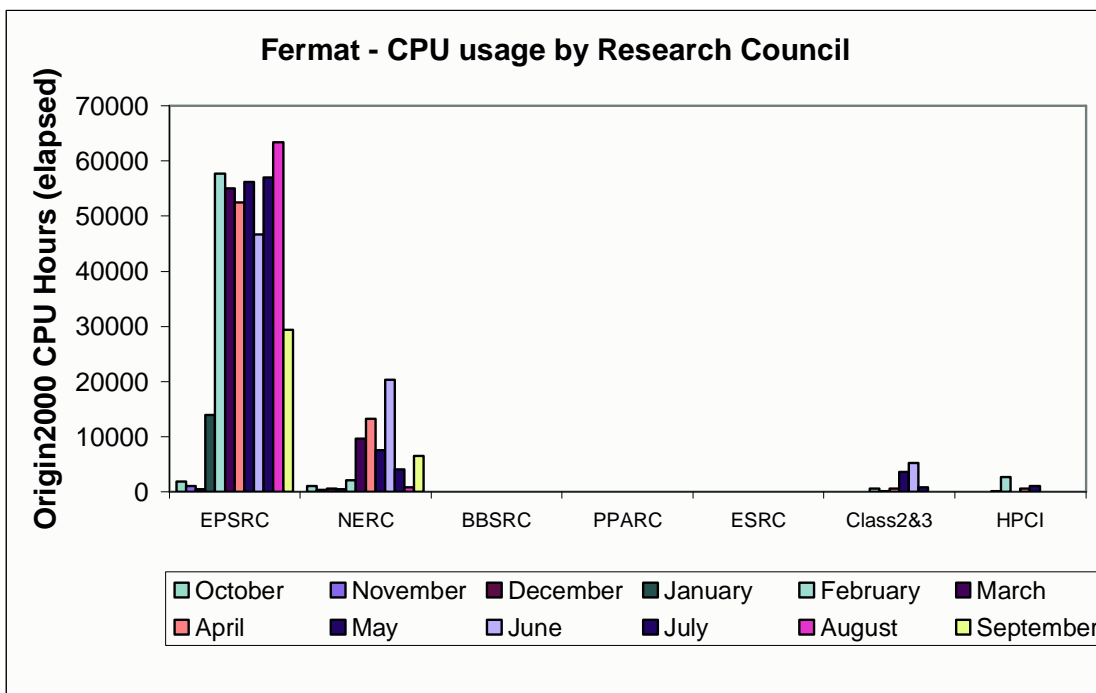
The largest proportion of the workload on Turing, 72%, was greater than 64 PEs in size.



The major allocation of the workload on Green, 61%, was greater than 64 PEs in size.



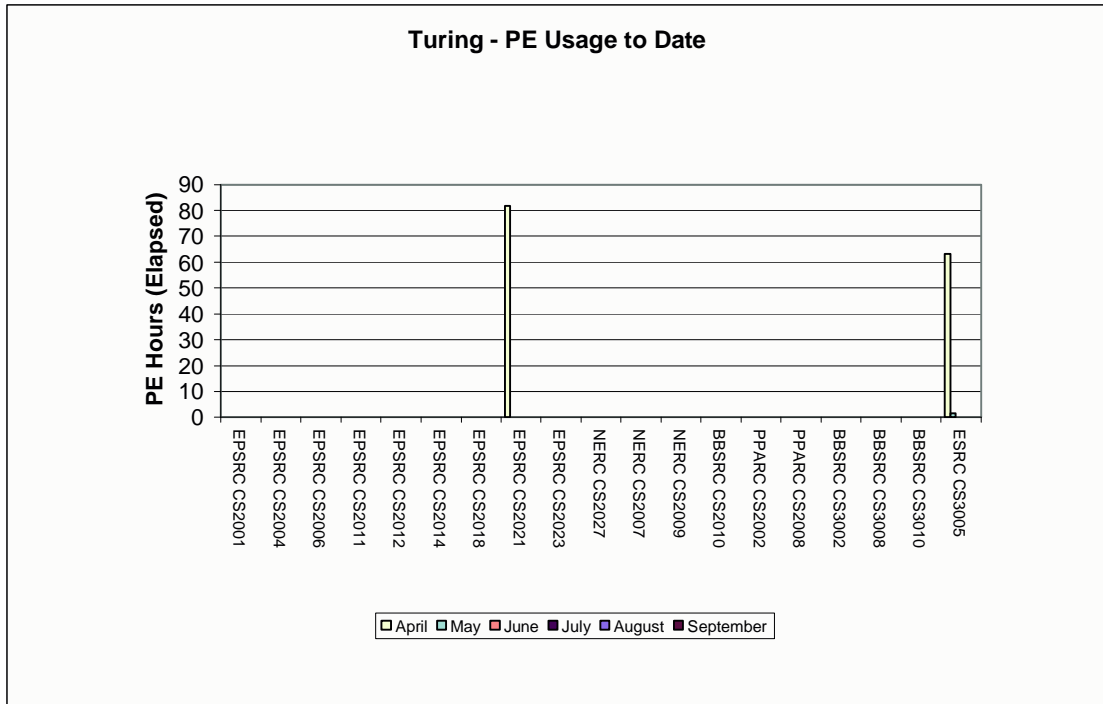
Turing PE usage is shown by Research Council during the past 12 months of service in the above chart.



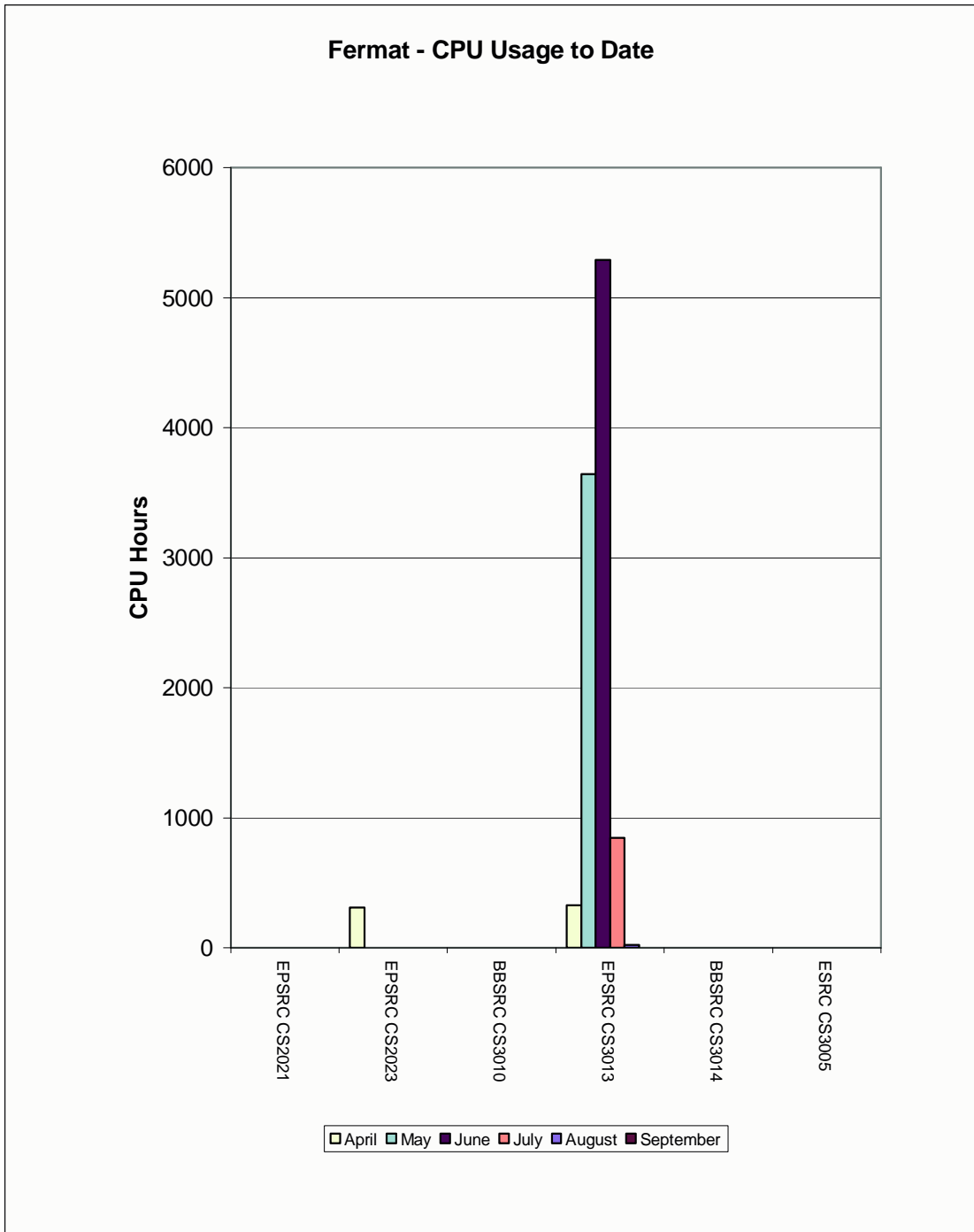
Origin 2000 CPU usage is shown by Research Council during the past 12 months of service in the above chart.

4.7 Class 2 & 3 Usage Charts

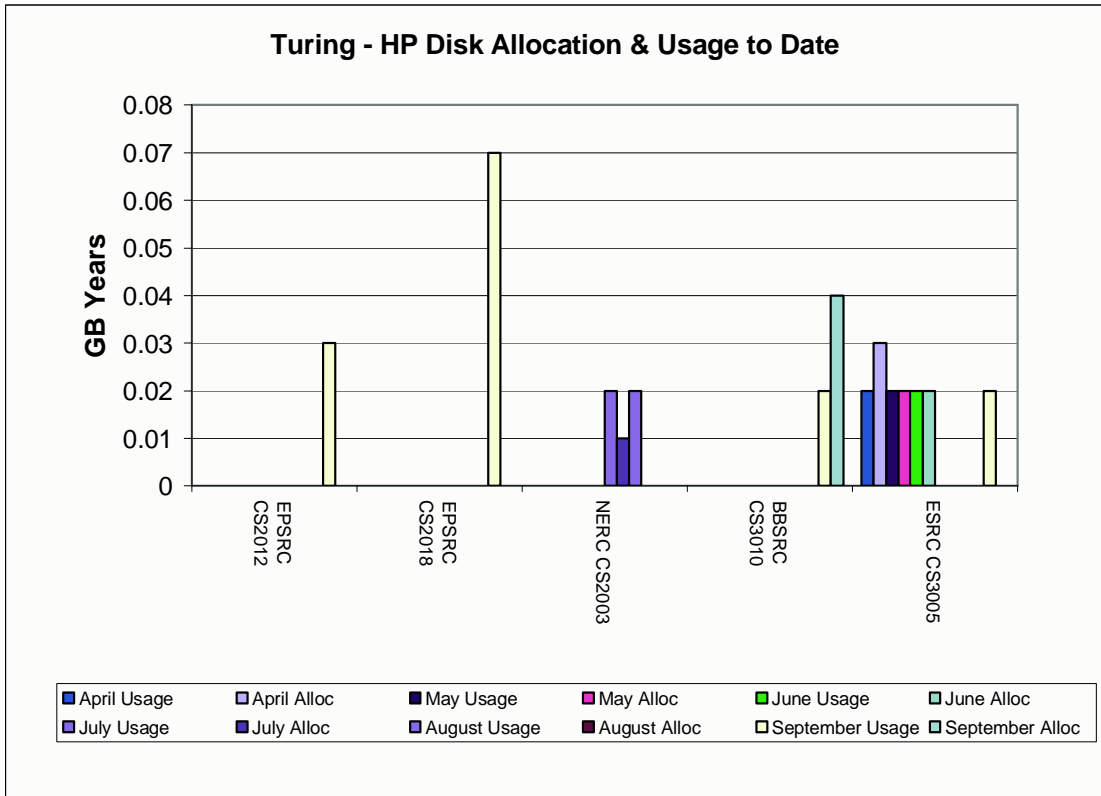
The next series of charts show the usage of the system by the class 2 & class 3 users. The usage is shown by project and identifies the Research Council of the individual projects.



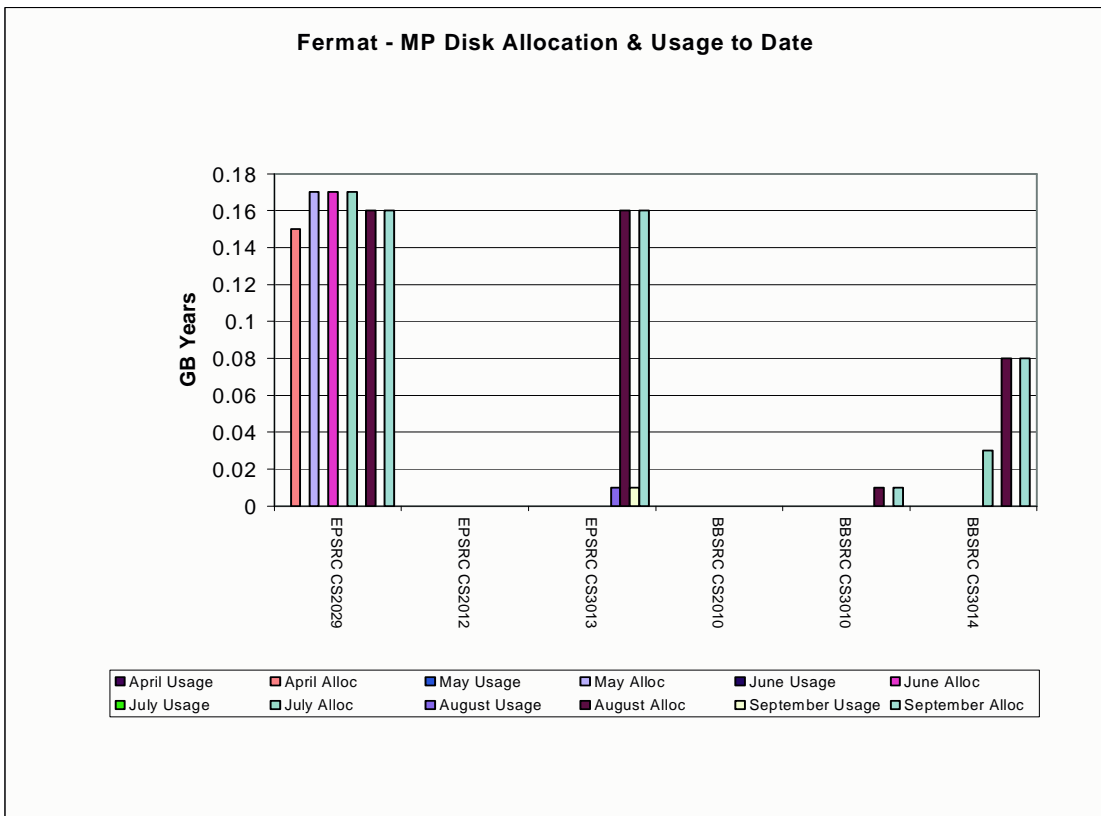
The above chart shows the most significant PE usage of the Turing system by class 2 and class 3 users.



The above chart shows the CPU usage of the Fermat system by class 2 and class 3 users.



The above chart shows the most significant disk allocations on the Turing system for class 2 and class 3 users.

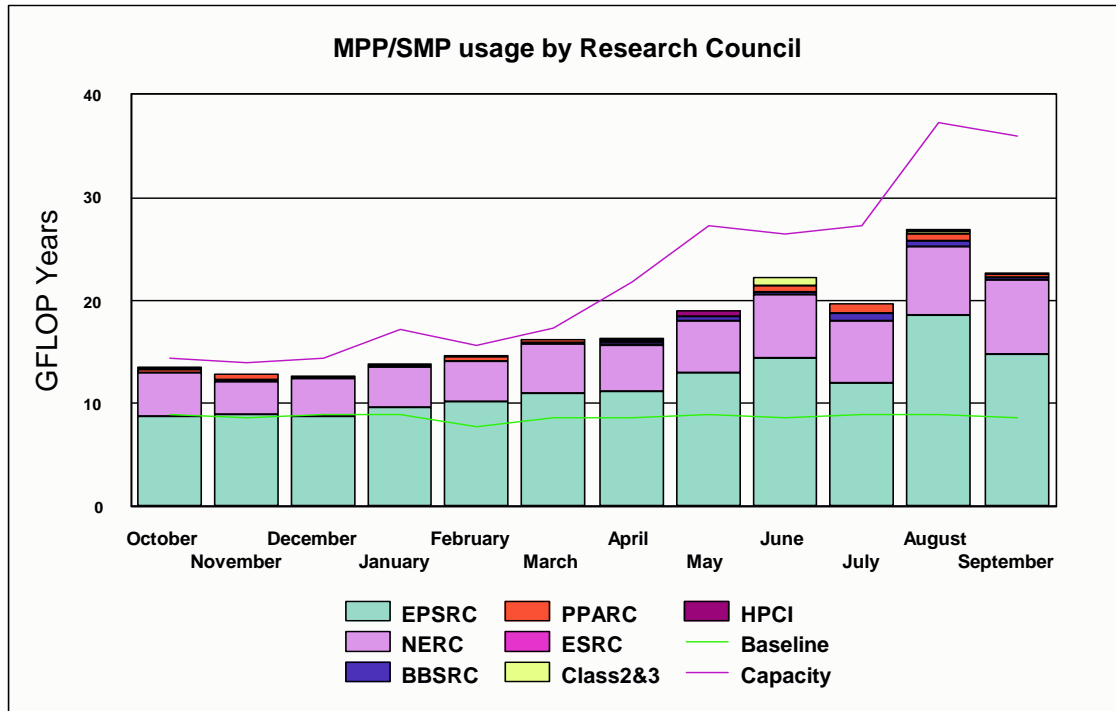


The above chart shows the most significant disk allocations on the Fermat system for class 2 and class 3 users. There is currently no HSM usage by class 2 and class 3 users.

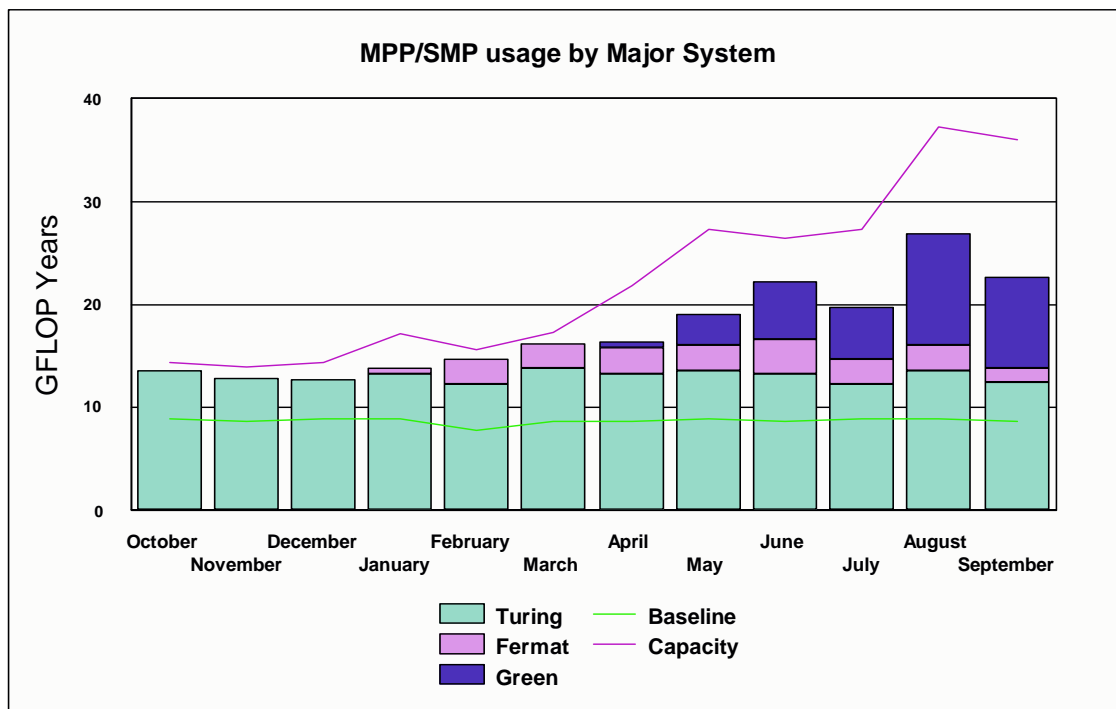
4.8 Charts of Historical Usage

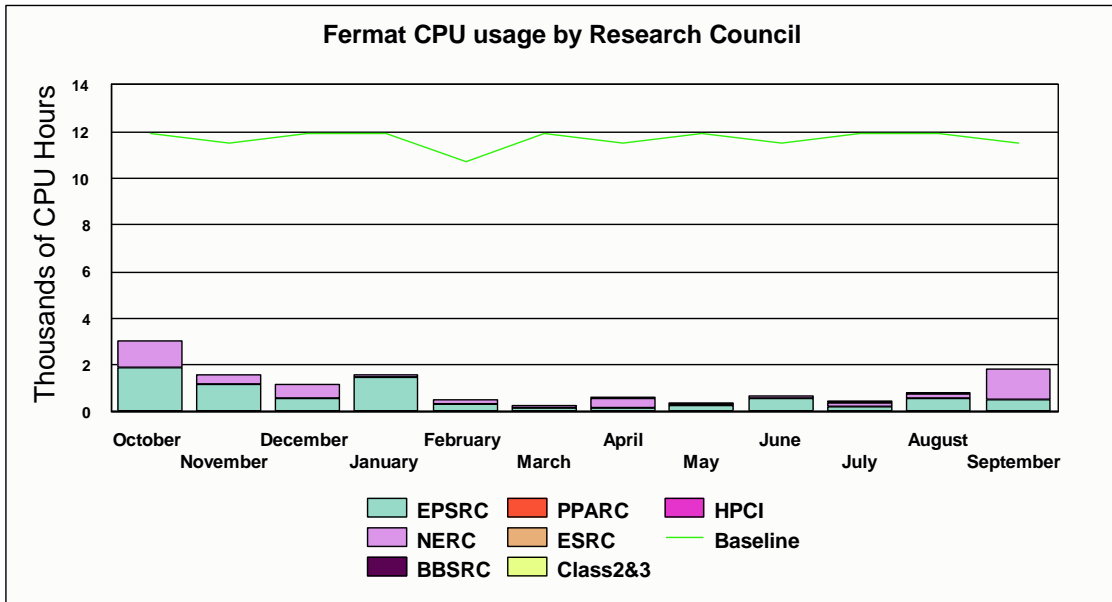
In all the Usage Charts, the baseline varies dependant on the number of days in each month, within a 365-day year.

The graph below shows the GFLOP Year utilisation on Turing and Fermat by Research Council for the previous 12 months; usage in July being reduced due to the outage for the major Green system upgrade.



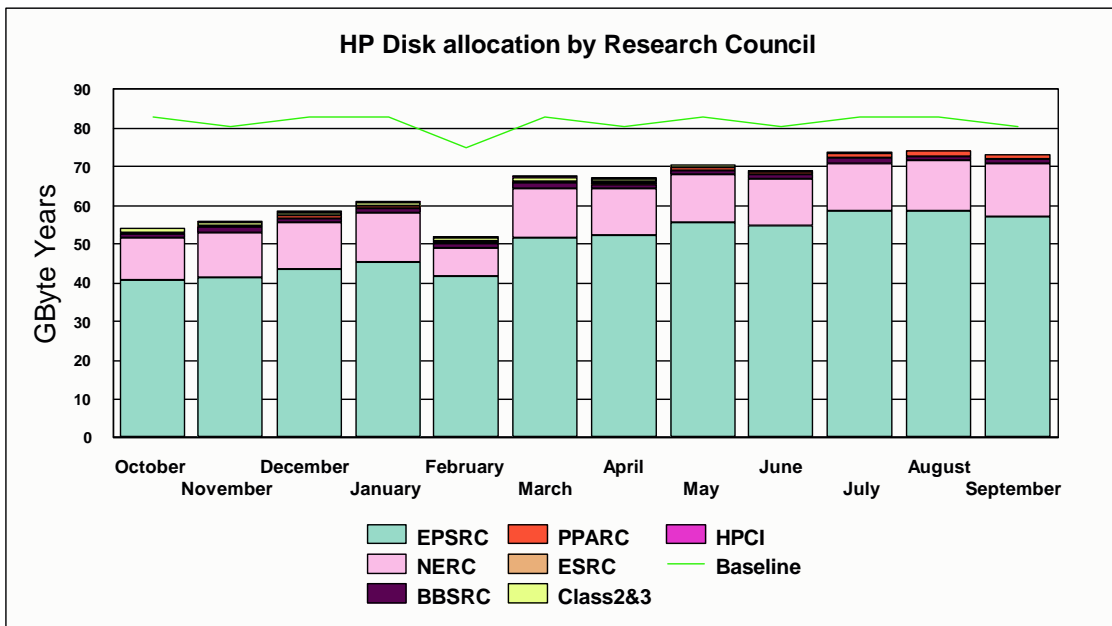
The graph below shows the historic SMP/MPP usage on the major systems, with the upgrades to Fermat showing in January 2001 and Green showing in April to September 2001.



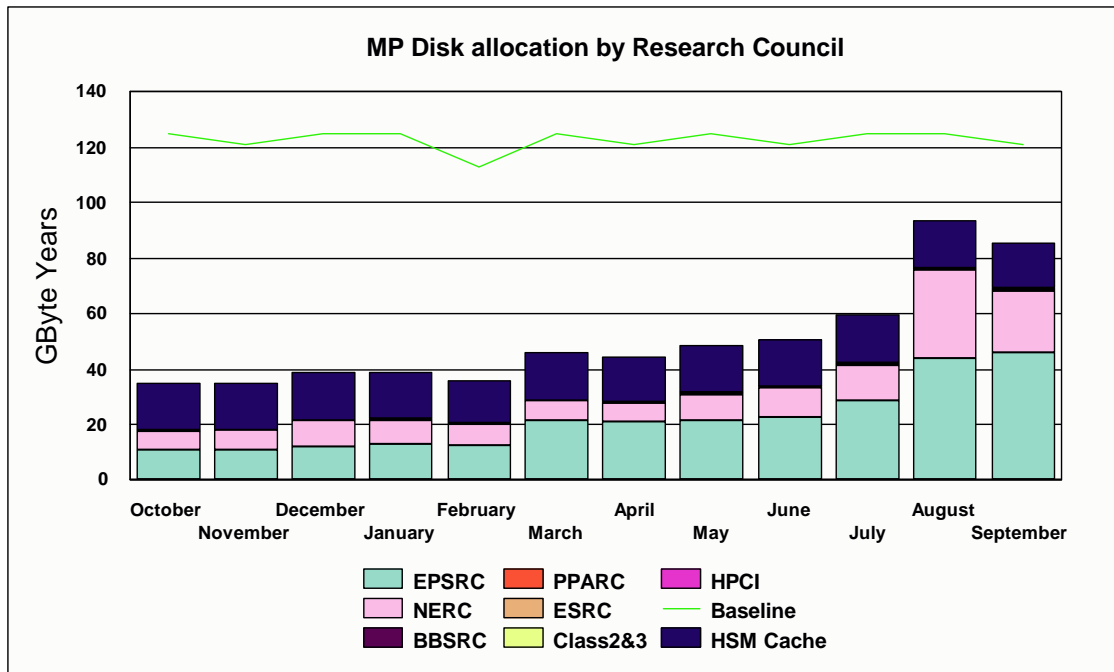


The above graph shows the historic interactive usage of the 'Baseline' Fermat system (equivalent to 16@250Mhz CPU's)

The next series of graphs illustrates the usage of the disk and HSM resources of the system.

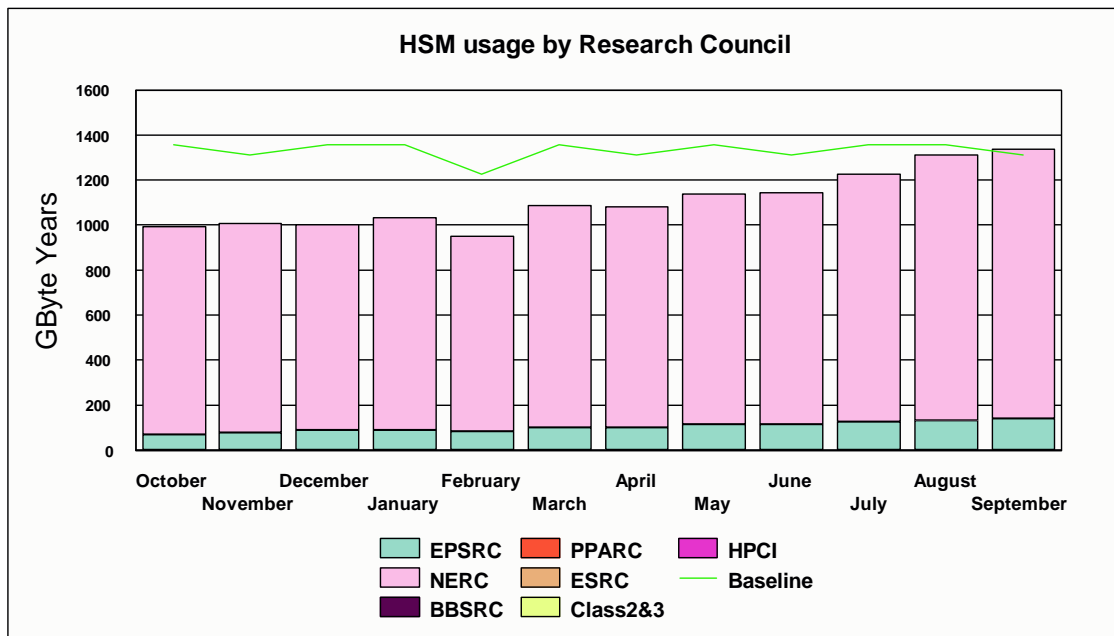


The preceding graph illustrates the historic allocation of the High Performance Disk on Turing, which is now approaching the Baseline level.

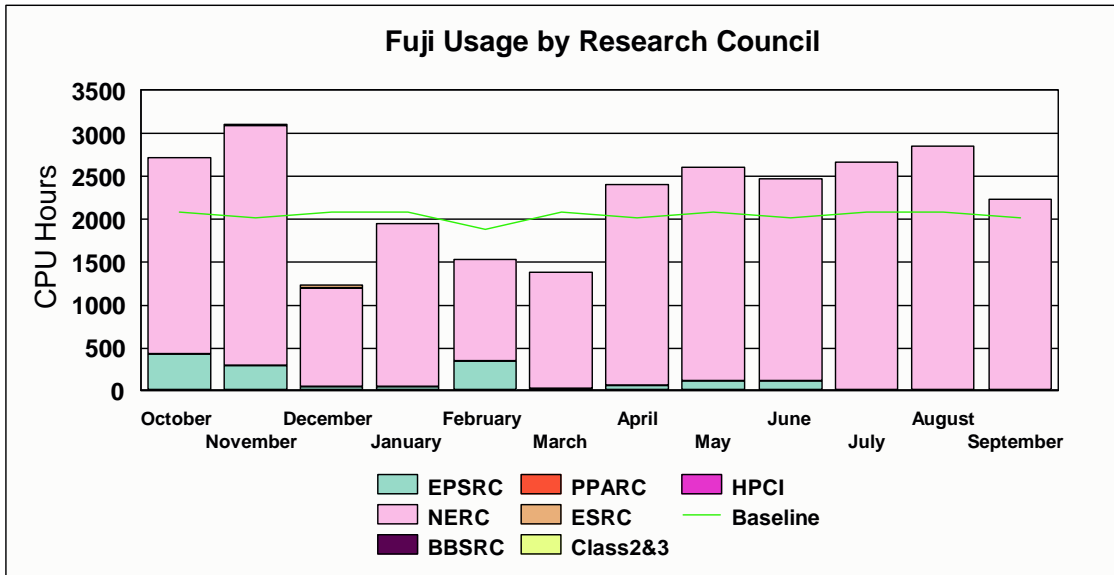


The graph above illustrates the historic allocation of the Medium Performance Disk on Fermat, which is now beginning to grow more rapidly with the growth in usage of both Fermat and Green.

The graph below shows the historic HSM usage by Research Council funded projects, now close to Baseline. The primary usage is for NERC.



The next chart shows the historic usage of the Fuji system.



The Fujitsu system usage was above baseline this month.

4.8 Guest System Usage Charts

There is currently no Guest System usage.

5. Service Status, Issues and Plans

5.1 Status

The service continues to run almost at full capacity.

During the month, 72% of the jobs run on Turing were larger than 64 PEs in size.

During the month, 61% of the jobs run on Green were larger than 64 PEs in size.

The batch usage of Green is currently at 45% of the machine's capacity.

5.2 Issues

The environmental issues, although no longer as evident, are still receiving Management attention.

5.3 Plans

Plans are underway for the implementation of a SAN solution to the service.

6. Conclusion

September 2001 saw the overall CPARS rating at Green with the baseline being exceeded by 48%.

The largest proportion of the workload continues to be of the larger job sizes.

Continued management attention will be given to maximise the throughput of the Service, whilst balancing as fairly as practicable the shares between Projects and jobs of the varying sizes.

Appendix 1 contains the accounts for September 2001

Appendix 2 contains the Percentage shares by Consortium for September 2001

Appendix 3 contains the Percentage shares by Research Council for September 2001

Appendix 4 contains the Training, Applications and Optimisation support figures to the end of September 2001

Appendix 5 contains a reference table of the Consortia name, the subject area and the PI name.

Appendix 1

The summary accounts for the month of September 2001 can be found at the URL below

<http://www.csar.cfs.ac.uk/admin/accounts/summary.shtml>

Appendix 2

Percentage PE time per consortia for Turing in September 2001		Percentage CPU time per consortia for Fermat in September 2001	
Consortia	% Machine Time	Consortia	% Machine Time
CSE002	23.25	CSE002	0.00
CSE003	0.41	CSE003	0.05
CSE007	0.00	CSE007	6.73
CSE021	0.00	CSE021	0.00
CSE023	0.00	CSE023	0.32
CSE025	0.00	CSE025	0.00
CSE030	0.02	CSE030	0.00
CSE051	0.00	CSE051	0.00
CSE055	0.00	CSE055	0.00
CSO057	0.04	CSO057	0.00
CSE006	0.04	CSE006	47.26
CSE026	0.66	CSE026	0.00
CSE004	6.12	CSE004	0.15
CSE013	4.94	CSE013	0.42
CSE014	0.00	CSE014	0.00
CSE016	0.00	CSE016	0.00
CSE027	0.00	CSE027	0.00
CSE040	0.00	CSE040	0.00
CSE041	0.00	CSE041	0.00
CSE043	0.00	CSE043	0.00
CSE052	1.07	CSE052	0.00
CSE053	0.05	CSE053	0.00
CSE056	0.00	CSE056	0.00
CSE008	0.00	CSE008	0.00
CSE009	8.70	CSE009	10.32
CSE024	1.56	CSE024	0.00
CSE033	0.00	CSE033	12.37
CSE035	5.02	CSE035	0.00
CSE019	0.00	CSE019	0.00
CSE020	0.00	CSE020	0.00
CSE066	0.71	CSE066	0.11
CSE034	0.00	CSE034	0.00
CSE036	0.00	CSE036	0.00
HPCI Southampton	0.00	HPCI Southampton	0.00
HPCI Daresbury	0.61	HPCI Daresbury	0.00
HPCI Edinburgh	0.02	HPCI Edinburgh	0.28
CSN001	1.27	CSN001	0.20
CSN003	33.93	CSN003	3.09
CSN005	0.00	CSN005	0.00
CSN006	5.87	CSN006	14.39
CSN007	0.00	CSN007	0.00
CSN010	0.00	CSN010	0.00
CSN011	0.01	CSN011	0.00
CSN012	0.00	CSN012	0.00
CSN015	2.05	CSN015	0.44
CSN017	1.77	CSN017	0.00
CSN036	0.00	CSN036	0.00
CSB001	1.45	CSB001	0.00
CSB002	0.06	CSB002	0.00
CSP002	2.14	CSP002	0.00
CSP003	0.00	CSP003	0.00
CSP004	0.00	CSP004	0.00
CS2018	0.00	CS2018	0.00
CS2021	0.00	CS2021	0.00
CS2023	0.00	CS2023	0.00
CS2026	0.00	CS2024	0.00
CS2027	0.00	CS2027	0.00
CS2029	0.00	CS2029	0.00
CS3001	0.00	CS3001	0.00
CS3002	0.00	CS3002	0.00
CS3005	0.00	CS3005	0.00
CS3007	0.00	CS3007	0.00
CS3008	0.00	CS3008	0.00
CS3010	0.00	CS3010	0.00
CS3012	0.00	CS3012	0.00
CS3013	0.00	CS3013	0.00
CS3014	0.00	CS3014	0.00

Appendix 2

Percentage disc allocation by Consortia for Turing in September 2001		Percentage disc allocation by Consortia for Fermat in September 2001	
Consortia	%Allocation	Consortia	%Allocation
CSE002	23.07	CSE002	7.44
CSE003	9.00	CSE003	3.56
CSE007	1.23	CSE007	0.59
CSE021	0.00	CSE021	0.00
CSE023	0.22	CSE023	13.56
CSE025	0.00	CSE025	0.00
CSE030	21.58	CSE030	30.18
CSE051	0.12	CSE051	0.13
CSE055	0.11	CSE055	0.00
CSE006	0.90	CSE006	0.48
CSE026	0.05	CSE026	0.00
CSE004	11.13	CSE004	3.57
CSE013	1.07	CSE013	0.25
CSE014	0.00	CSE014	0.00
CSE016	0.14	CSE016	0.00
CSE027	0.05	CSE027	1.78
CSE040	0.00	CSE040	0.00
CSE041	0.05	CSE041	0.00
CSE043	0.04	CSE043	0.12
CSE052	0.34	CSE052	0.00
CSE053	0.11	CSE053	0.00
CSE056	0.00	CSE056	0.00
CSE008	0.00	CSE008	0.00
CSE009	6.74	CSE009	0.59
CSE024	0.40	CSE024	0.04
CSE033	0.05	CSE033	2.97
CSE035	0.79	CSE035	0.00
CSE019	0.00	CSE019	0.00
CSE020	0.00	CSE020	0.00
CSE066	0.72	CSE066	0.82
CSE034	0.00	CSE034	0.00
CSE036	0.03	CSE036	0.01
HPCI Southampton	0.00	HPCI Southampton	0.00
HPCI Daresbury	0.11	HPCI Daresbury	0.06
HPCI Edinburgh	0.11	HPCI Edinburgh	0.12
CSN001	11.24	CSN001	11.89
CSN003	2.37	CSN003	1.78
CSN005	0.00	CSN005	0.00
CSN006	4.50	CSN006	1.19
CSN007	0.00	CSN007	0.00
CSN010	0.00	CSN010	0.00
CSN011	0.45	CSN011	0.00
CSN012	0.00	CSN012	0.17
CSN015	0.14	CSN015	17.36
CSN017	0.01	CSN017	0.12
CSN036	0.05	CSN036	0.00
CSB001	0.05	CSB001	0.00
CSB002	1.46	CSB002	0.12
CSP002	0.67	CSP002	0.00
CSP003	0.03	CSP003	0.04
CSP004	0.79	CSP004	0.59
CS2018	0.00	CS2018	0.00
CS2026	0.00	CS2026	0.00
CS2029	0.00	CS2029	0.23
CS3001	0.00	CS3001	0.00
CS3002	0.00	CS3002	0.00
CS3005	0.00	CS3005	0.00
CS3010	0.05	CS3010	0.00
CS3012	0.00	CS3012	0.00
CS3013	0.00	CS3013	0.23
CS3014	0.00	CS3014	0.12

<u>Research Council</u>	<u>% usage</u>	
EPSRC	10.25	
HPCI	0	
NERC	89.62	
BBSRC	0	
ESRC	0	
PPARC	0	

Appendix 3

Percentage PE usage on Turing by Reserch Council for September 2001			Percentage CPU usage on Fermat by Reserch Council for September 2001		
Research Council	% Usage		Research Council	% Usage	
EPSRC	52.59		EPSRC	81.88	
HPCI	0.63		HPCI	0.00	
NERC	43.13		NERC	18.12	
BBSRC	1.51		BBSRC	0.00	
ESRC	0.00		ESRC	0.00	
PPARC	2.14		PPARC	0.00	

Percentage Disc allocated on Turing by Research Council for September 2001			Percentage Disc allocated on Fermat by Research Council for September 2001		
Research Council	% Allocated		Research Council	% Allocated	
EPSRC	77.96		EPSRC	66.59	
HPCI	0.22		HPCI	0.17	
NERC	18.74		NERC	32.35	
BBSRC	1.57		BBSRC	0.12	
ESRC	0.00		ESRC	0.00	
PPARC	1.49		PPARC	0.64	

Percentage usage of HSM by Consortium for September 2001	
Consortium	% Usage
CSE002	0.69
CSE003	0.10
CSE023	0.03
CSE030	2.18
CSE004	5.01
CSE013	0.06
CSE027	0.13
CSE041	0.07
CSE024	1.79
CSE033	0.12
CSE035	0.05
CSN001	17.80
CSN003	62.00
CSN015	9.82

Appendix 4

The following tables show the training and support resource usage by the consortias in person days to the current month. Optimisation support for September totalled 10.5 man days.

Code	PI	Subject	Application Support for September 2001	Total Application Support from July 2000	Optimisation Support for September 2001	Total Optimisation Support from July 2000	Total Support Used	Training Used
Cse002	Dr Phil Lindan	Support for the UKCP		10.75			142.75	-
Cse003	Prof. Ken Taylor	HPC Consortiums 98- 2000		6		15.5	24.5	6
Cse004	Dr Neil Sandham	UK Turbulence						2
Cse006	Dr Patrick Briddon	Covalently Bonded Materials						
Cse007	Dr Matthew Foulkes	Quantum Many Body Theory					1	2
Cse008	Dr Mark Vincent (Hillier)	Model Chemical Reactivity						
Cse009	Dr Ben Slater (Catlow)	HPC in Materials Chemistry		6		3	9	
Cse010	Dr John Williams	Free Surface Flows					15.95	
Cse011	Dr John Williams	Open Channel Flood Plains					2.18	
Cse013	Prof Michael Leschziner	Complex Engineering Flows						3
Cse014	Dr Cassiano de Oliverira (Goddard)	Probs in Nuclear Safety						
Cse016	Dr Stewart Cant	Turbulent Combustion						
Cse017	Dr Kai Luo	Large Eddy Simulation and Modelling of Buoyant Plumes and Smoke Spread in Enclosures						
Cse018	Dr Stewart Cant	Turbulent Flames						
Cse019	Dr Jason Lander (Berzins)	ROPA						
Cse020	Dr Marek Szularz	Symmetric Eigenproblem						
Cse021	Dr Julie Staunton	Magentisim						1
Cse022	Mr Niall Branley (Jones)	Turbulent Flames						

Cse023	Allen	Liquid Crystalline Materials						
Cse024	Dr Robert Allan (Tennyson)	ChemReact 98-2000						-
Cse025	Dr Niels Rene Walet(Bishop)	Nuclear Theory Programme						1.5
Cse026	Dr Maureen Neal	Molecular Dynamics						
Cse027	Dr M Imregun	Excitation Mechanisms						
Cse028	Prof. P.W. Bearman	Bridge Design						
Cse029	Dr David Aspley (Leschziner)	Validation of Turbulence Models						
Cse030	Prof M Cates (VIPAR)	HPC for Complex Fluids		21		5	51	7
Cse033	Dr M Imregun	Tubomachinery core compressor						
Cse034	Dr Paul Durham	R&D of liner/non-linear systems						
Cse035	Dr Stephen Jenkins	Ab Initio Simulations						
Cse036	Prof Iain Duff	R&D of linear/non-linear systems						
Cse040	Dr Ken Badcock	-						
Cse041	Dr M Imregun	Flutter and Noise Generation						
Cse043	Dr J J R Williams	Numerical Simulation of flow over a rough bed						4
Cse051	Prof B L Gyorffy	Ab initio calculations of magnetic anisotropies in Fe						
Cse052	Miss Francesca Di Mare (Hayes)	Heat Transfer in Gas Turbine Combustors						
Cse053	Prof M A Leschziner	Coupling Rans Near-Wall Turbulence Models with Large Eddy Simulation Strategies						
Cse055	Dr Julia Staunton	Ab-initio theory of magnetic anisotropy in transition metal ferromagnets						
Cse056	Dr Mehmet Imregun	Aerothermoelasticity modelling of air riding seals for large gas turbines						
Cse066	Dr Keir Novik	Novel clay-polymer nanocomposites using diversity-discovery methods: synthesis, processing and testing						

Csn001	Mrs Beverly de Cuevas (Webb)	HPCI Global Ocean Consortium		1			3	1
Csn002	Dr Mark Vincent (Hillier)	Pollutant Sorption on Mineral Surf						
Csn003	Dr Lois Steenman-Clark (O'Neill)	UGAMP						4
Csn005	Dr Huw Davies	Constraining Earth Mantle					27	6
Csn006	Dr John Brodholt (Price)	Density Functional Methods						
Csn007	Dr John Brodholt (Price)	Density Functional Methods						
Csn008	Hulton	Sub-Glacial Process						
Csn009	Dr Roger Proctor							
Csn010	Dr Jason Lander (Mobbs)	Flow over Complex terrain						
Csn011	Dr Ed Dicks (Thorpe)	Exchange of Polluted Air						
Csn012	Prof Tennyson	fuji user						
Csn013	Dr L Steenman-Clark (Voke)	Large-Eddy Simulation Extended by Extreme Value Theory for the Prediction of Dispersion, Concentration Threshold Boundaries and Field Connectivity						
Csn014	Prof Llewellyn-Jones	A new Data Assimilation Scheme to optimise the information on the surface-atmosphere interface from satellite observations of Top-of-the-Atmosphere Brightness Temperature						
Csn015	Dr Roger Proctor	Atlantic Margin Metocean Project		2			2	3
Csn017	Dr Antony Payne	Stability of the Antarctic Ice Sheet						2
Csn036	Prof Keith Haines	Assimilation of Altimeter, Radiometer and in situ data into the OCCAM Model. Analysis of water properties and transports.						
Csb001	Dr David Houldershaw (Goodfellow)	Macromolecular Interactions		1.5			3.5	2
Csb002	Dr Adrian Mulholland (Danson)	Stability of Enzymes at high temp						

Csb003	Dr John Carling (Williams)	Anguilliform Swimming						
Csp002	Dr Sandra Chapman	Nonlinear process in solar system and astrophysical plasmas						4
Csp003	Prof Andrew Lyne	Computing Resources for Precision timing of Millisecond Pulsars		1			2	4
Csp004	Prof K L Bell	A Programme for Atomic Physics for Astrophysics at Queen's University, Belfast (2001 – 2005)						
Css001	Dr I J Turton	Human Systems Modelling						
Css002	Dr Robert Crouchley	Dropout in panel surveys						2
Hpcid	Dr Robert Allan							1
Hpcie	Dr David Henty							
Hpcis	Dr Denis Nicole							
ukhec	Ms K Jaffri							2
Cs2001	Dr Sudhir Jain	3D Ising Spin Glass						
Cs2002	Dr Ingrid Stairs (Lyne)	Millisecond Pulsars					0.25	
Cs2004	Dr A. Paul Watkins	Internal Combustion Engine						
Cs2006	Prof. Walter Temmerman	Superconductivity & Magnetism						
Cs2007	Choularton	Precipitation in the Mountains						1
Cs2008	Dr Matthew Genge	Extraterrestrial Mineral Surfaces					7.91	
Cs2009	Dr Roger Proctor	Atlantic Margin Metocean Project						
Cs2010	Dr Christopher Dempsey	Helical membrane-lytic peptides						
Cs2011	Dr D Drikakis	Transition & Turbulence in Physiological Flows						
Cs2012	Prof Ning Qin	Monotone Integrated Large Eddy Simulation						1.5
Cs2014	Dr Vladimir Karlin	Dynamics of intrinsically unstable premixed flames						2
Cs2015	Mr Pablo Tejera-Cuesta	Nonlinear Methods in Aerodynamics						1.5
Cs2016	Dr Jim Miles	Investigation of Scaline Properties of Hierarchical Micromagnetic Models						

Cs2017	Mr Markus Eisenbach	Ab initio calculations of magnetic anisotropies in Fe inclusions in Cu						
Cs2018	Mr Maxim Chichkine	Study of defect clusters in silicon for sub-micron technologies						
Cs2019	Dr Guy H Grant	Theoretical studies of flavoproteins						
Cs2020	Prof John Barker	Predicting the applicability of Aquifer Storage Recovery (ASR) in the UK						
Cs2021	Dr A R Mount	A Computational Study of the Luminescence of Substituted Indoles						1
Cs2022	Dr Philippa Browning	Numerical simulation of forced magnetic reconnection						2
Cs2023	Prof W Ewen Smith	The use of DFT methods for the accurate prediction of the Ramen spectrum of large molecules						
Cs2024	Prof J G Doyle	Modelling of late-type stellar chromospheres						
Cs2026	Dr R J Greenall	Molecular dynamics simulations of AT-tract DNA						
Cs2027	Dr Anthony Kay	Mathematical Model of the Circulation of Lake Baikal						
Cs2028	Dr James F Annett	Numerical Tests of Disorder Effects in D-Wave Superconductors						
Cs2029	Prof B L Gyorffy	Ab-initio calculations of unconventional electronic, magnetic and lattice properties of magnitudes						
Cs2030	Prof G J Morgan	Spin Diffusion in Magnetic Multilayers						
Cs3001	Mr John Andrew Staveley	Helical Coherent Structures					0	3
Cs3002	Dr Keir Novik	Simulations of DNA oligomers						2
Cs3003	Dr Eric Chambers	Band III peptide fragments						
Cs3004	Prof Nick Avis	Computational Steering and Interactive Virtual Environments						1
Cs3005	Mr Behrouz Zarei	Simulation of Queuing Networks						3
Cs3006	Mr F Li	Quantifying Room Acoustic Quality						1

Cs3007	Emma Finch	Development of a 3D Crustal Lattice Solid Model		7		5	12	-
Cs3008	Dr B J Alsberg	Development of a 3D QSAR method based on quantum topological descriptors						
Cs3009	Dr D Flower	Epitope Prediction Methods based on molecular dynamics simulation						
Cs3010	Dr K Kemsley	Investigation of electromyographic recordings of muscle activity during chewing, and of relationships with perceived flavour and texture, in model and real food systems					-	1
Cs3012	Prof Jim Austin	Evaluation of binary neural networks on a vector parallel processor				3	3	2
Cs3013	Prof Rasmita Raval	Structure and function of Chiral Bioarrays: A fundamental approach to proteomic devices						
CS014	Dr John Brooke	Enabling UK Academic Grid Application Development and Testing						

Appendix 5

Code	PI	Subject	Subject Area
Cse002	Dr Nicolas Harrison (Gillan)	Support for the UKCP	Physics
Cse003	Prof. Ken Taylor	HPC Consortiums 98- 2000	Physics
Cse004	Dr Neil Sandham	UK Turbulence	Engineering
Cse006	Dr Patrick Briddon	Covalently Bonded Materials	Materials
Cse007	Dr Matthew Foulkes	Quantum Many Body Theory	Physics
Cse008	Dr Mark Vincent (Hillier)	Model Chemical Reactivity	Chemistry
Cse009	Dr Ben Slater (Catlow)	HPC in Materials Chemistry	Chemistry
Cse010	Dr John Williams	Free Surface Flows	Engineering
Cse011	Dr John Williams	Open Channel Flood Plains	Engineering
Cse013	Dr David Aspley (Leschziner)	Complex Engineering Flows	Engineering
Cse014	Dr Cassiano de Oliverira (Goddard)	Probs in Nuclear Safety	Engineering
Cse016	Dr Stewart Cant	Turbulent Combustion	Engineering
Cse018	Dr Stewart Cant	Turbulent Flames	Engineering
Cse019	Dr Jason Lander (Berzins)	ROPA	Information Technology
Cse020	Dr Marek Szularz	Symmetric Eigenproblem	Information Technology
Cse021	Dr Julie Staunton	Magentisim	Physics
Cse022	Mr Niall Branley (Jones)	Turbulent Flames	Engineering
Cse023	Allen	Liquid Crystalline Materials	Robin Pinning
Cse024	Dr Robert Allan (Tennyson)	ChemReact 98-2000	Chemistry
Cse025	Dr Niels Rene Walet (Bishop)	Nuclear Theory Programme	Physics
Cse026	Dr Maureen Neal	J90 move	
Cse027	Dr M Imregun	J90 move	
Cse028	Prof. P.W. Bearman	J90 move	
Cse029	Dr David Aspley (Leschziner)	J90 move	Engineering
Cse030	Prof M Cates	HPC for Complex Fluids	Physics
Cse031	Brebbia	J90 move	
Cse033	Dr M Imregun	Tubomachinery core compressor	Chemistry
Cse034	Dr Paul Durham	R&D of liner/non-linear systems	Mathematics
Csn001	Mrs Beverly de Cuevas (Webb)	HPCI Global Ocean Consortium	
Csn002	Dr Mark Vincent (Hillier)	Pollutant Sorption on Mineral Surf	
Csn003	Dr Lois Steenman-Clark (O'Neill)	UGAMP	
Csn005	Dr Huw Davies	Constraining Earth Mantle	
Csn006	Dr John Brodholt (Price)	Density Functional Methods	
Csn007	Dr John Brodholt (Price)	Density Functional Methods	
Csn008	Hulton	Sub-Glacial Process	
Csn009	Dr Roger Proctor		
Csn010	Dr Jason Lander (Mobbs)	Flow over Complex terrain	
Csn011	Dr Ed Dicks (Thorpe)	J90 move	
Csb001	Dr David Houldershaw (Goodfellow)	Macromolecular Interactions	
Csb002	Dr Adrian Mulholland (Danson)	Stability of Enzymes at high temp	
Csb003	Dr John Carling (Williams)	J90 move	
Css001	Dr Stan Openhaw	Human Systems Modelling	
Css002	Dr Robert Crouchley	Dropout in panel surveys	
Hpcid	Dr Robert Clough		
Hpcie	Dr David Henty		
Hpcis	Dr Denis Nicole		
Cs2001	Dr Sudhir Jain	3D Ising Spin Glass	
Cs2002	Dr Ingrid Stairs (Lyne)	Millisecond Pulsars	
Cs2003	Mr Tom Coulthard	Holocene Sediment Fluxes	
Cs2004	Dr A. Paul Watkins	Internal Combustion Engine	
Cs2005	Mr Sean Walsh	Arabidopsis Genome	
Cs2006	Prof. Walter Temmerman	Superconductivity & Magmetisim	
Cs2007	Chouartan	Precipitation in the Mountains	
Cs2008	Dr Matthew Genge	Extraterrestrial Mineral Surfaces	
Cs3001	Mr John Andrew Staveley	Helical Coherent Structures	