CSAR Service

Consolidated Management Report

4th Quarter 2004

<u>Management Summary</u>

This is the consolidated Management report for the fourth quarter 2004 of the CSAR HPC facility for UK Academia and Industry, which enables World-Class research and development.

The number of users has grown to a total of 471 to date.

The workload on both the Origin 3000 Green and the Altix 3700 Newton has been fairly evenly spread across the mid- to high-end ranges of PEs during the fourth quarter of this year.

CSAR has been granted an 18-month extension of service contract until June 30th 2006. With this extension CfS implemented a further technology refresh introducing a 256 processor Itanium-2 (Madison) based SGI Altix, now enhanced to 512 processors with 1 Terabyte of memory.

CfS remains active in the UK Grid Forum.

Introduction

This Management Report includes a section for each of the main service functions:

1. Service Quality
2. HPC Services
3. Science Applications Support Services
4. Training & Education Services
5. User Registration & New User Services
6. Value-Added Services

Each section includes a status report for the period, including notable achievements and problems, also noteworthy items for the next period.

1   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.

1.1   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. Overall, the CPARS Performance Achievement for the 4th quarter 2004 was satisfactory (see Table 3), i.e. Green measured against the CPARS performance targets.

CSAR Service - Service Quality Report - Actual Performance Achievement

Service Quality Measure	Jan	Feb	March	April	May	June	July	Aug	Sept	Oct	Nov	Dec
HPC Services Availability												
Availability in Core Time (% of time)	97.49%	98.16%	98.51%	89.39%	94.21%	97.49%	97.97%	100%	99.52%	97.08%	98.50%	99.50%
Availability out of Core Time (% of time)	98.88%	97.9%	99.48%	91.90%	99.73%	97.85%	100%	99.2%	99.80%	98.67%	98.78%	99.2%
Number of Failures in month	5	4	3	5	3	4	2	2	2	3	4	2
Mean Time between failures in 52 week rolling period (hours)	265	243	786	541	447	365	342	316	294	264	237	225
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	<2	<2	<2	<2	<3	<2	<2	<1	<2	<3	<1	<0.5
Administrative Queries - Max Time to resolve 95% of all queries	<0.5	<0.5	<0.5	<0.5	<0.5	<1	<0.5	<0.5	<1	<1	<0.5	<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	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<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	10	10	10	10	10	10
System Maintenance - no. of sessions taken per system in the month	2	2	2	2	2	2	2	2	2	2	2	2

Table 2

Notes:

1. HPC Services Availability has been calculated using the following formula, based on the relative NPB performance of Fermat, Green and Newton at installation:

   [Fermat availability x 40/ (40+233+343)] + [Green availability x 233/(40+233+343)] + [Newton availability x 343/(40+233+343)]

2. Mean Time Between Failures for Service Credits is formally calculated from a rolling 12-month period.

Table 3 gives Service Credit values for each month to date. These are 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	Jan	Feb	March	April	May	June	July	Aug	Sept	Oct	Nov	Dec
HPC Services Availability												
Availability in Core Time (% of time)	0.078	0.078	0.039	0.195	0.195	0.078	0.078	-0.058	-0.039	0.078	0.039	-0.039
Availability out of Core Time (% of time)	0	0.078	0	0.039	0	0.078	-0.047	0	-0.047	0	0	0
Number of Failures in month	0.0004	0.008	0	0.0004	0.0	0.008	0	0	0	0.008	0.008	0
Mean Time between failures in 52 week rolling period (hours)	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
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	0	0	0	0.016	0	0	-0.016	0	0.016	-0.016	-0.019
Administrative Queries - Max Time to resolve 95% of all queries	-0.019	-0.019	-0.019	0	-0.019	-0.016	-0.019	-0.019	-0.016	-0.01551	-0.019	-0.016
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	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-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	0	0	0	0	0
System Maintenance - no. of sessions taken per system in the month	0	0	0	0	0	0	0	0	0	0	0	0
Monthly Total & overall Service Quality Rating for each period:	0.01	0.05	-0.01	0.09	0.07	0.05	-0.02	-0.07	-0.07	0.02	-0.02	-0.06

Quarterly Service Credits:	0.05	0.21	-0.15	-0.05

Annual Service credit	0.06

Table 3

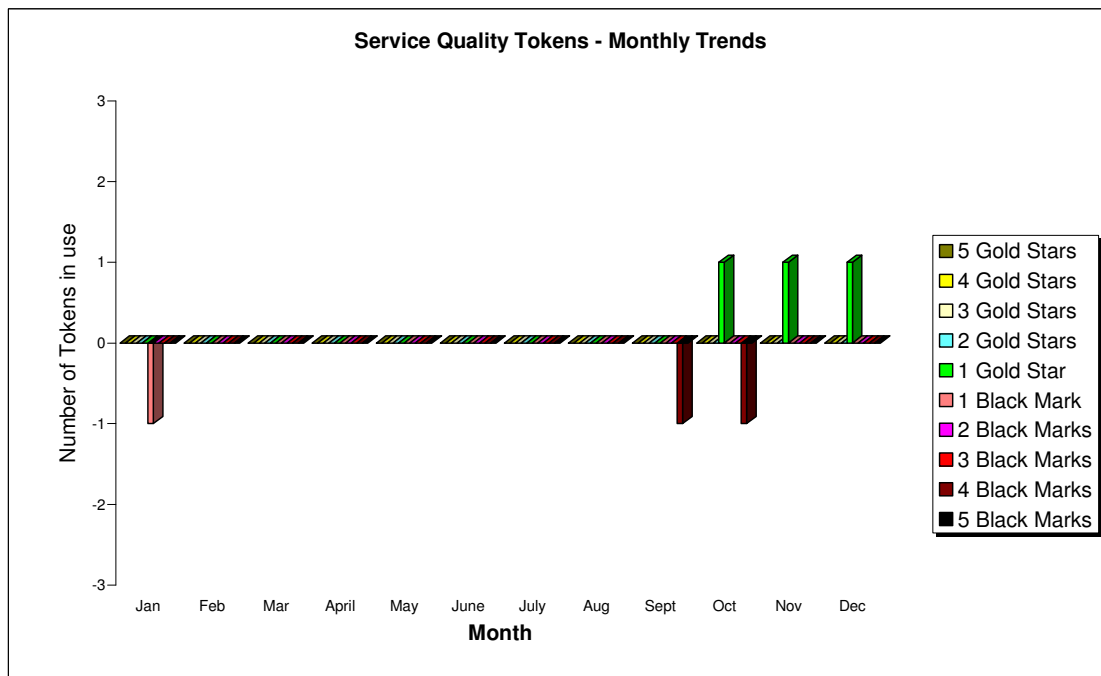Overall, system availability has steadily improved since the previous Quarter.

1.2   No. of Registered Users

The current position at the end of the quarter is that there are 471 registered users of the CSAR Service.

Total number of Users Registered
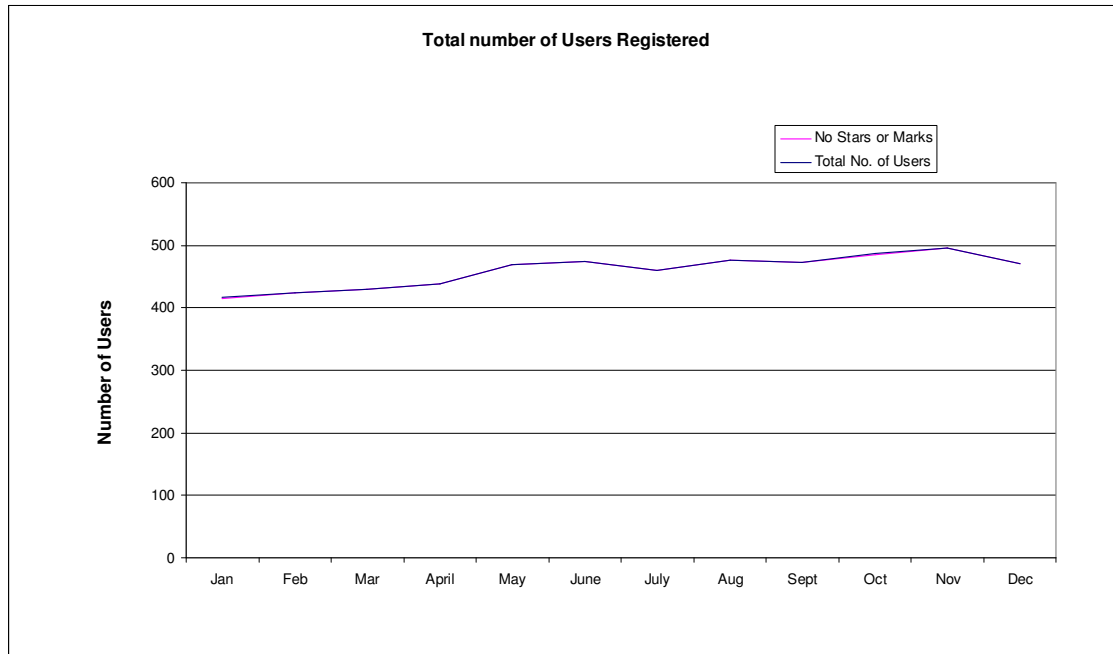
1.3   Service Quality Tokens

The graph below illustrates the monthly usage trend of Service Quality Tokens:

Over the course of the quarter the position is that as a management tool the Service Quality Tokens have been available to enable the users to provide qualitative feedback about all aspects of the service. This feedback is used as a mechanism to initiate change in the service where appropriate.

At the end of the quarter one user had allocated one gold star to the service:

SUMMARY OF SERVICE QUALITY TOKEN USAGE

No of Stars or Marks	Consortia	Date Allocated	Reason Given
1 gold star	cs3025	17/12/2004	Assistance with porting code

2   HPC Services Usage

Usage information is given in tabular form, and in graphical format. The system usage information covers:

- CPU usage
- User Disk allocation
- HSM/tape usage

 This is illustrated in a number of graphs including;

a)   SMP (Altix/Origin) Usage by month, showing usage each month of CPU (GFLOP-Years as per NPB), split
     by Research Council and by system. Overlaid horizontal lines show the overall Capacities.

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 and overall Capacity are shown by overlaid
     horizontal lines.

c)   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.

d)   HSM/Tape Usage 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.
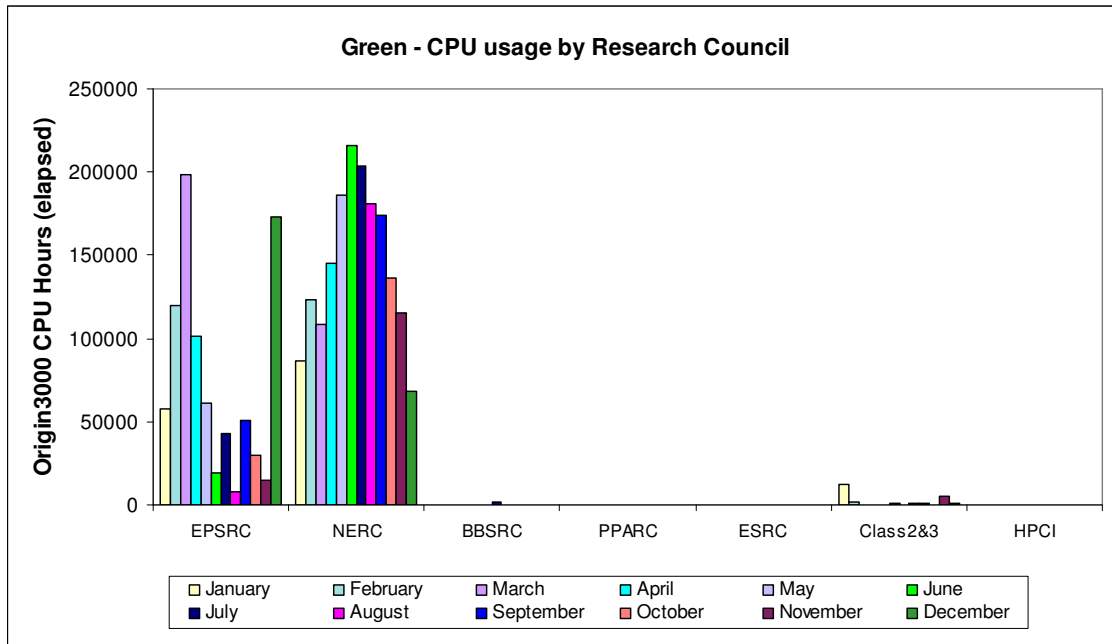
2.1   Service Usage Charts

The graphs below show recent monthly CPU, disk and HSM allocations and usage.

Newton - CPU usage by Research Council
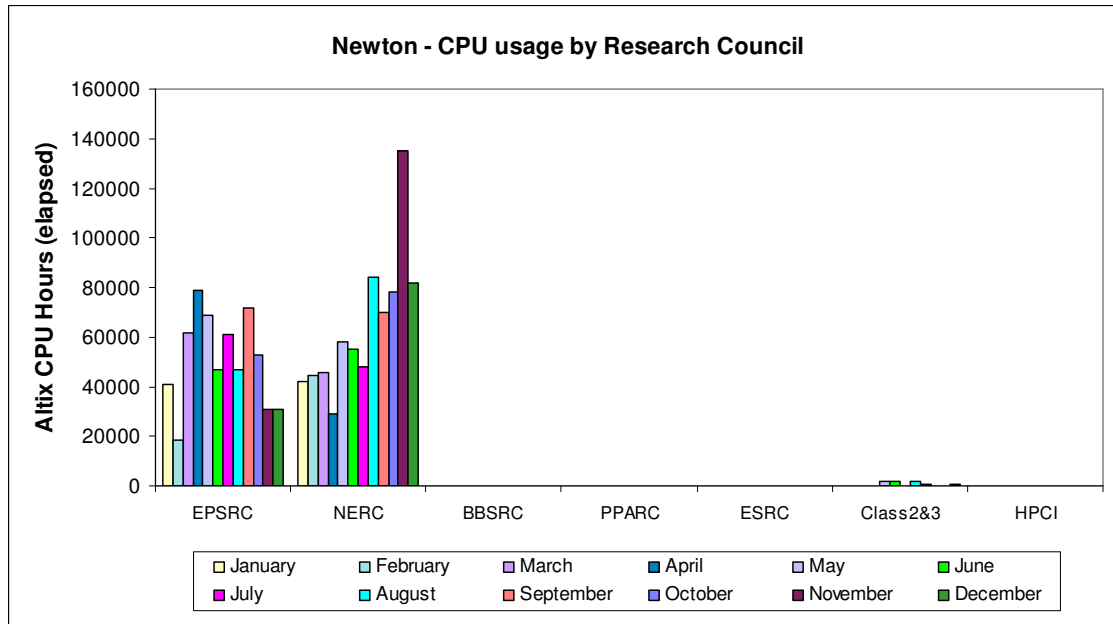
Usage of the SGI Altix 3700 system Newton is shown by Research Council in the above graph.

Fermat - CPU usage by Research Council
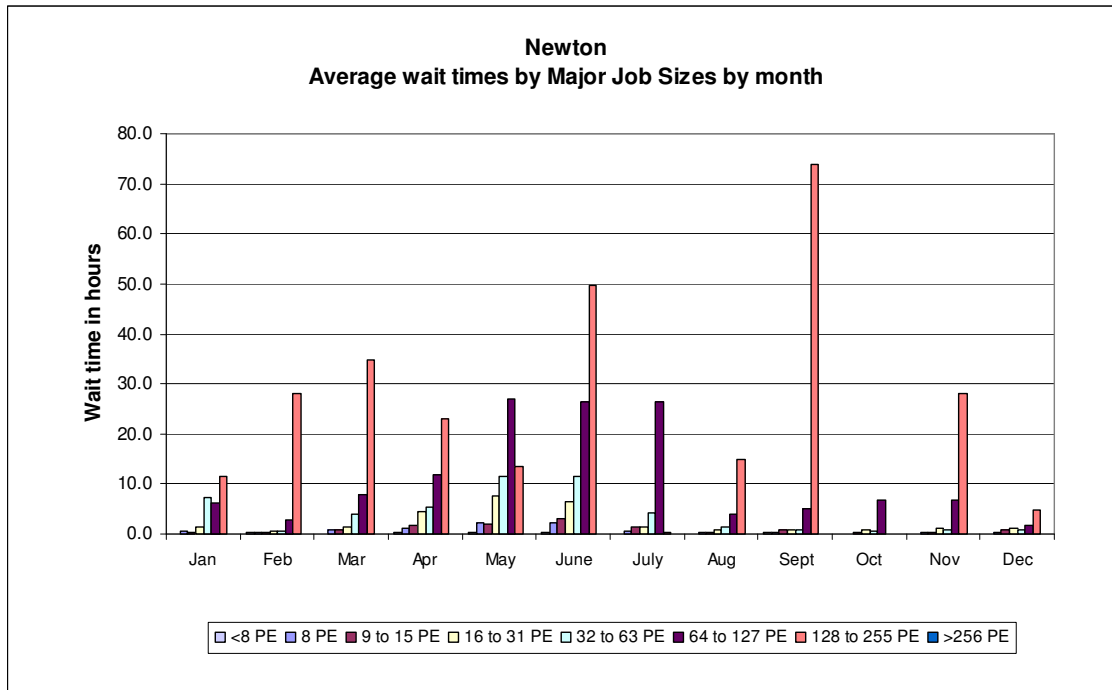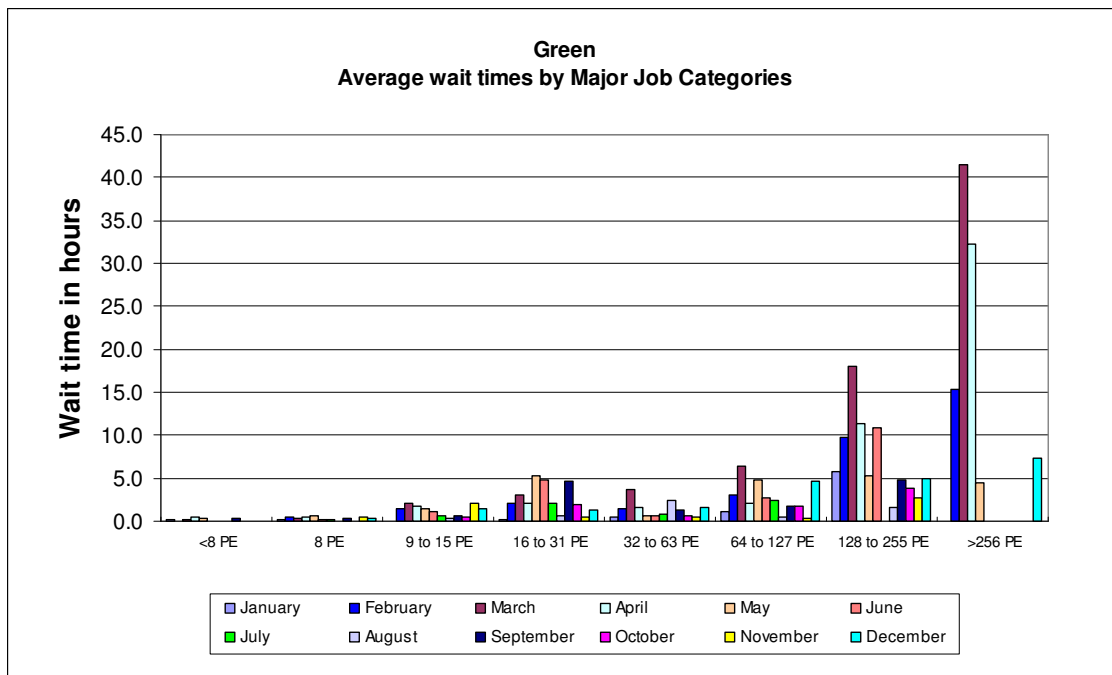
Green - CPU usage by Research Council
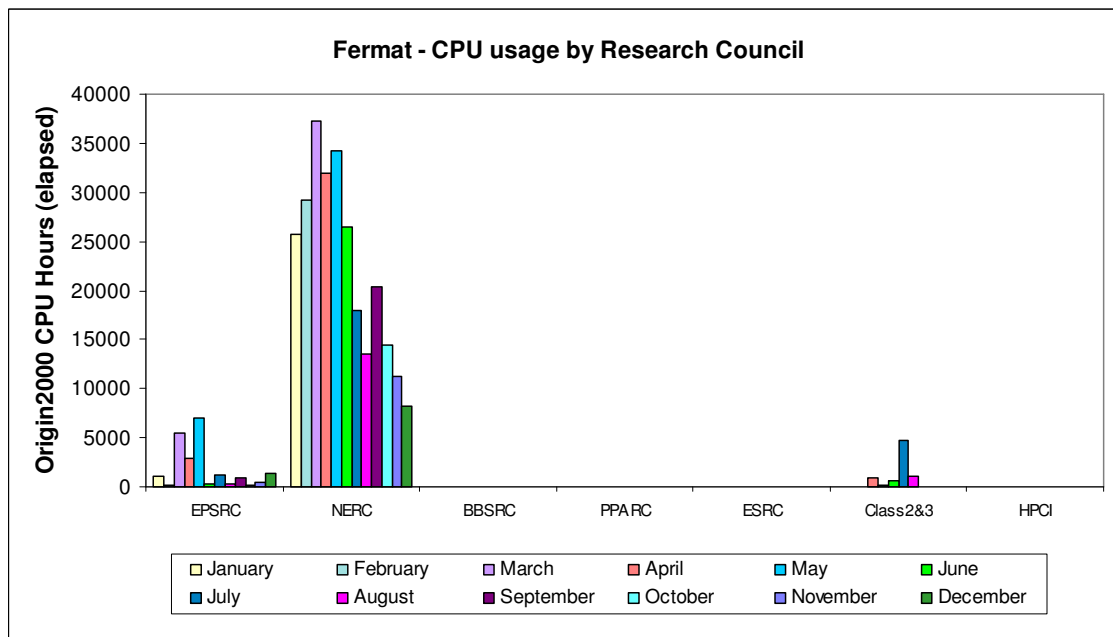
Usage of the two batch SGI Origin systems, Fermat and Green, is shown by Research Council during the last 12 months of service in the preceding two charts.
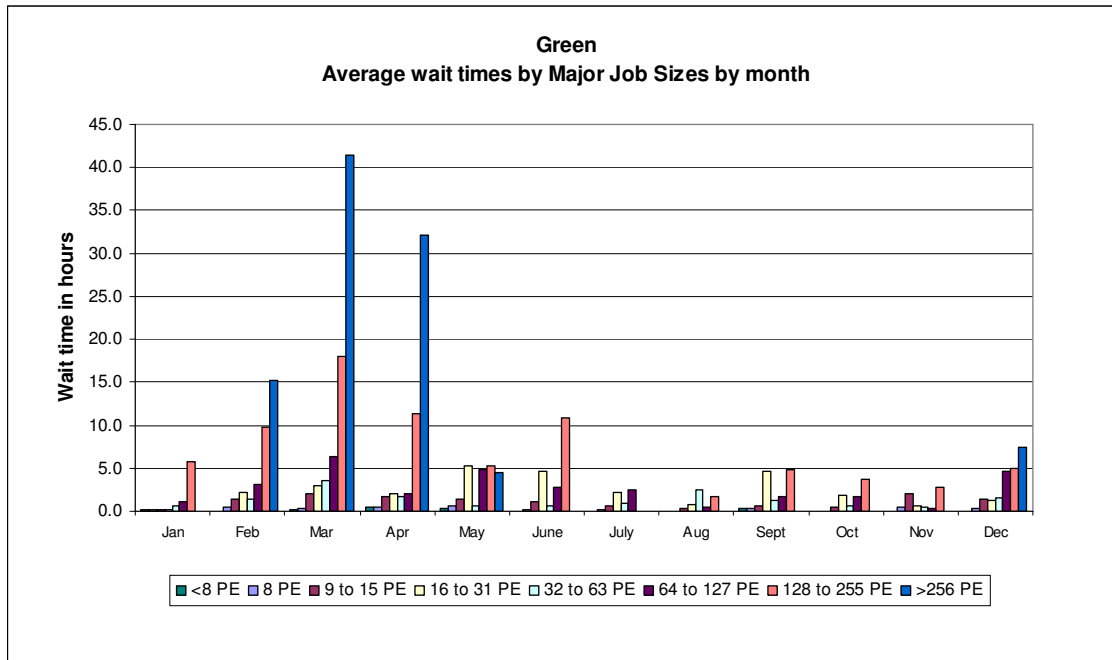
Newton
Average wait times by Major Job Categories
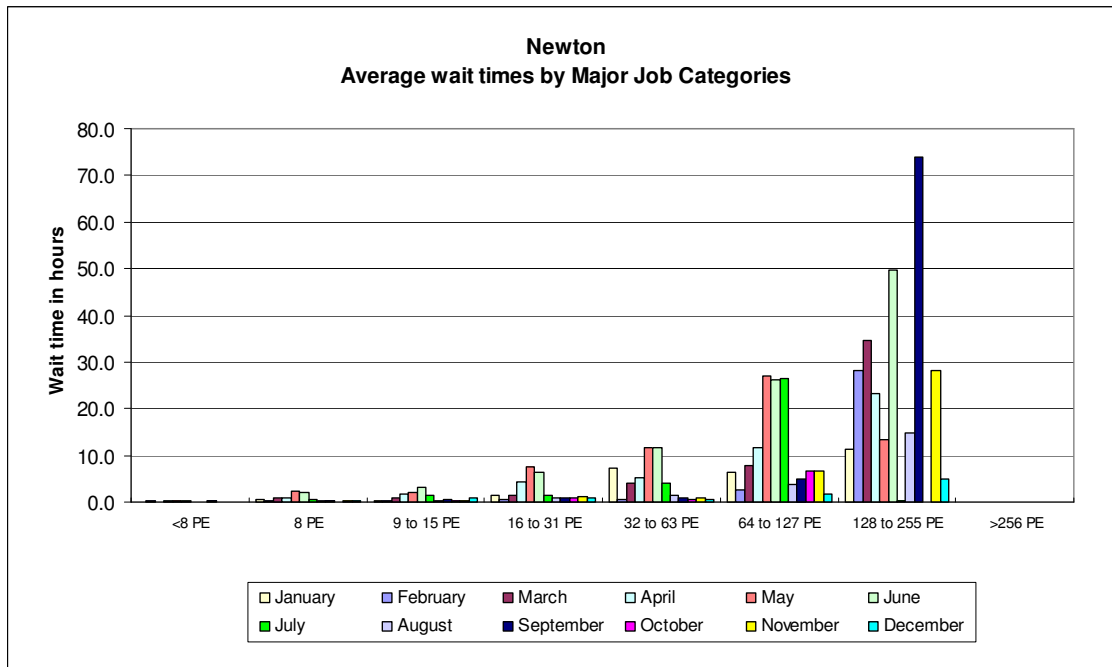
The above chart, and the one below, shows the wait time trend in hours on the Altix 3700 Newton.

Newton
Average wait times by Major Job Sizes by month

The following two charts show average wait times in hours for the quarter on the Origin 3000 Green.

Green
Average wait times by Major Job Categories

**Green
Average wait times by Major Job Sizes by month**

Legend: ■ <8 PE ■ 8 PE ■ 9 to 15 PE □ 16 to 31 PE □ 32 to 63 PE ■ 64 to 127 PE ■ 128 to 255 PE ■ >256 PE
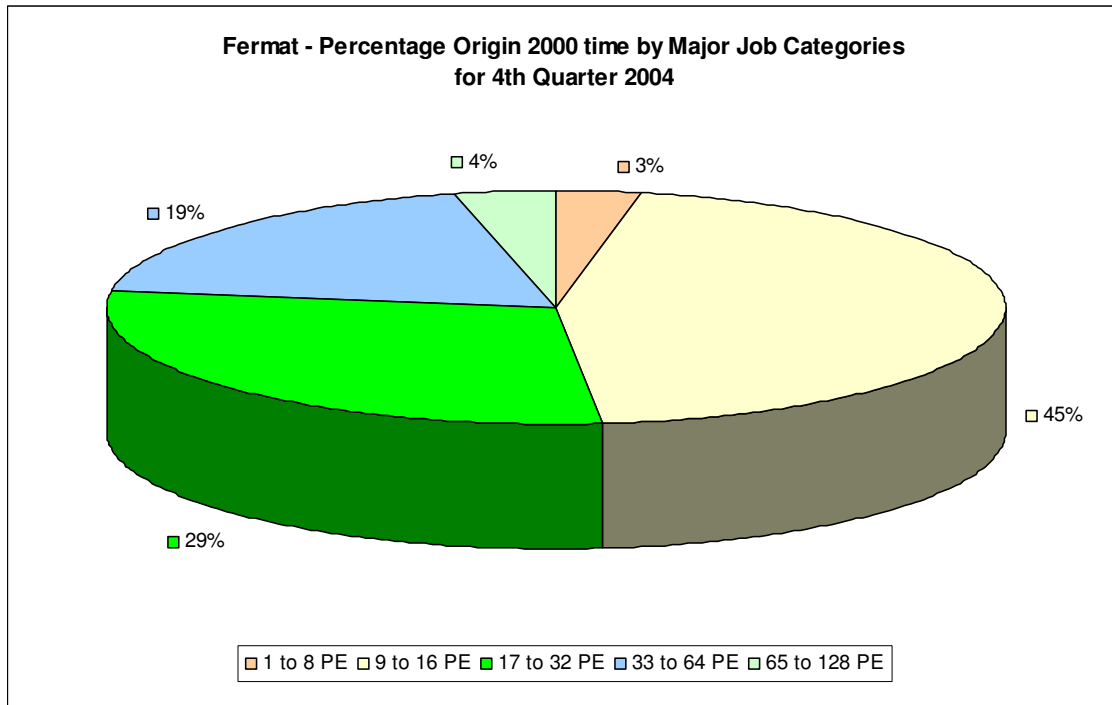
The next series of four charts show the percentage CPU time utilisation by the major job categories on the Green, Fermat and Newton systems for the 4th quarter 2004.

**Green - Percentage Origin 3000 time by Major Job Categories
for 4th Quarter 2004**

Legend: □ 1 to 8 PE □ 9 to 16 PE ■ 17 to 32 PE □ 33 to 64 PE □ 65 to 128 PE ■ 129 to 256 PE □ >256 PE
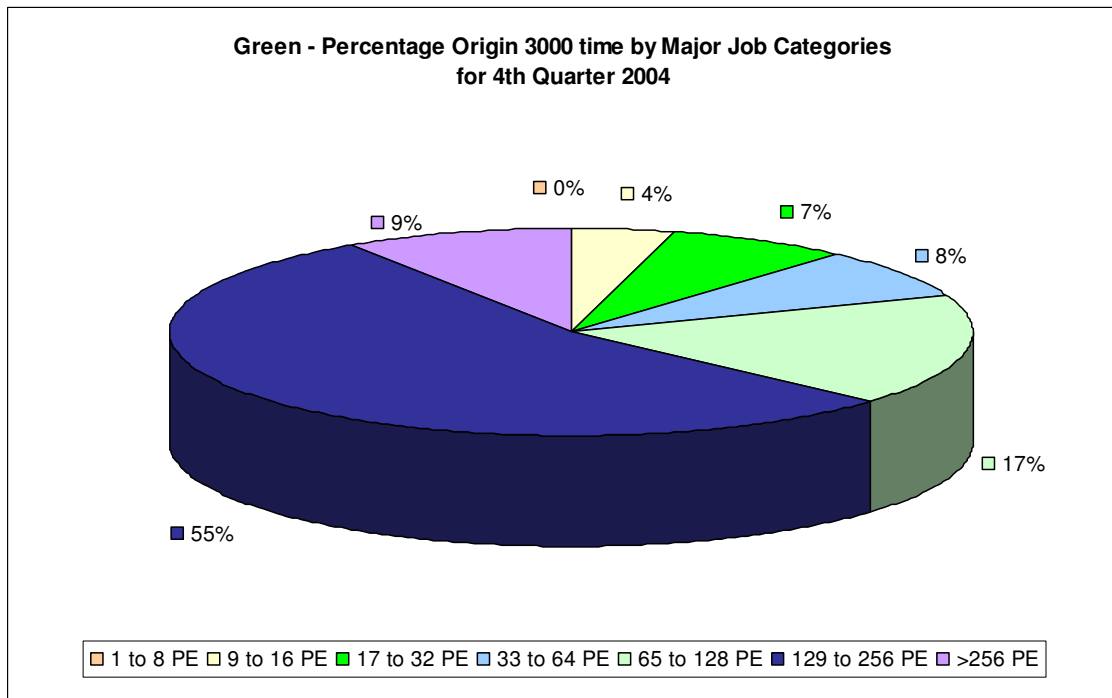
On Green, the 129 to 256 PE range has seen the greatest percentage of workload during this quarter.

**Fermat - Percentage Origin 2000 time by Major Job Categories
for 4th Quarter 2004**

- 4%
- 3%
- 19%
- 45%
- 29%

☐ 1 to 8 PE ☐ 9 to 16 PE ☐ 17 to 32 PE ☐ 33 to 64 PE ☐ 65 to 128 PE

On Fermat there was a varied spread of work across the entire range of PEs.

**Newton - Percentage Altix 3700 time by Major Job Categories
for 4th Quarter 2004**

- 3%
- 1%
- 14%
- 38%
- 18%
- 26%

☐ 1 to 8 PE ☐ 9 to 16 PE ☐ 17 to 32 PE ☐ 33 to 64 PE ☐ 65 to 128 PE ☐ 129 to 256 PE
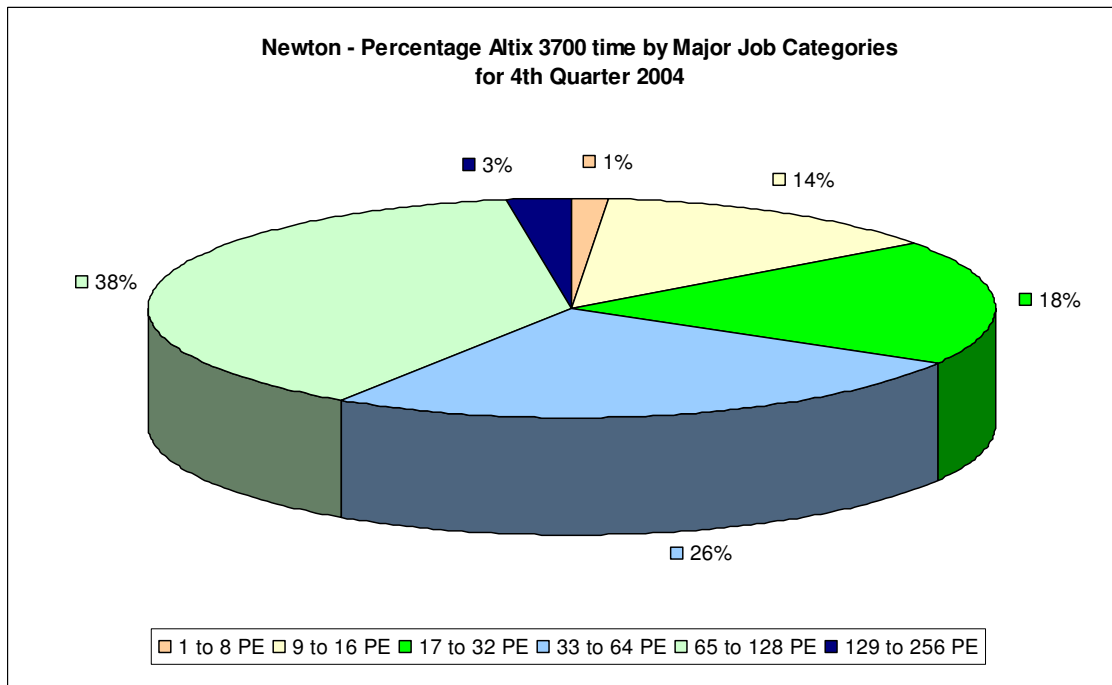
There was a good spread of work across Newton during the fourth quarter.

Job Size Trend on Green
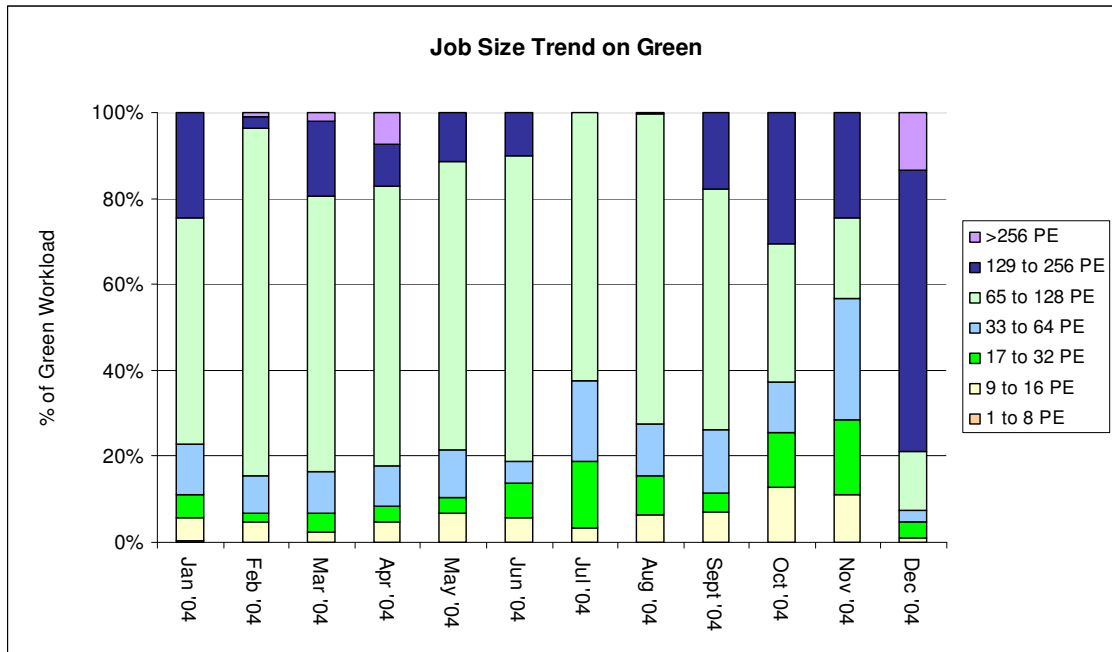
Usage on Green tended more to be in the mid- to high-range of PEs during the 4th quarter.

Job Size Trend on Fermat
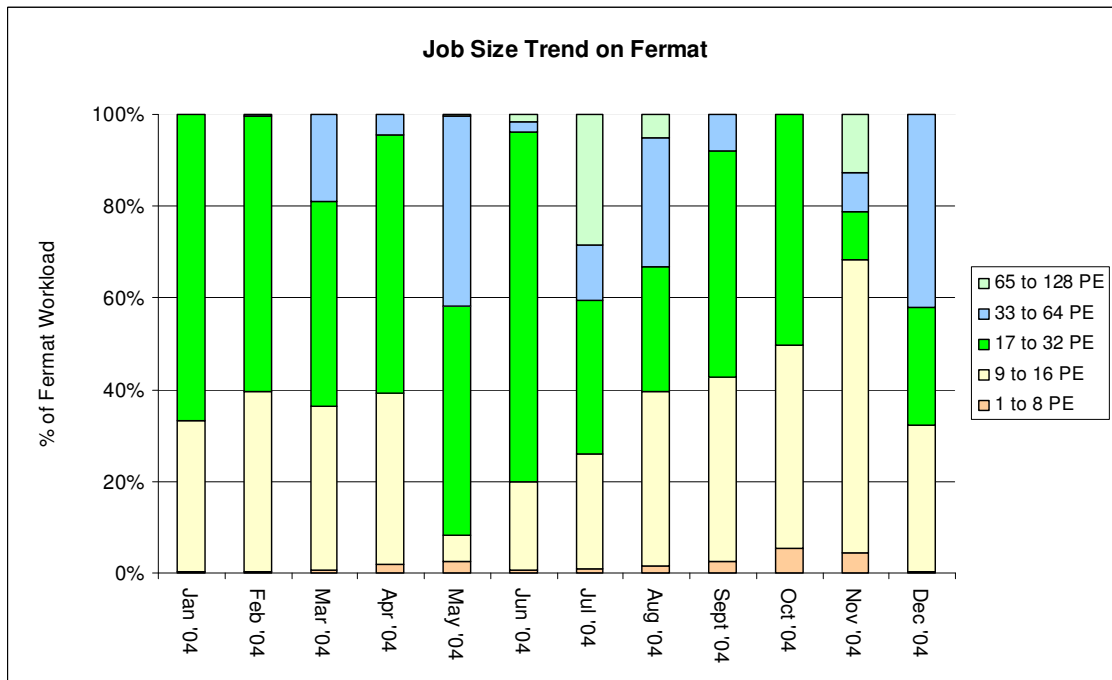
The workload on Fermat for this quarter was also spread fairly evenly across the mid-range of PEs.

Job Size Trend on Newton
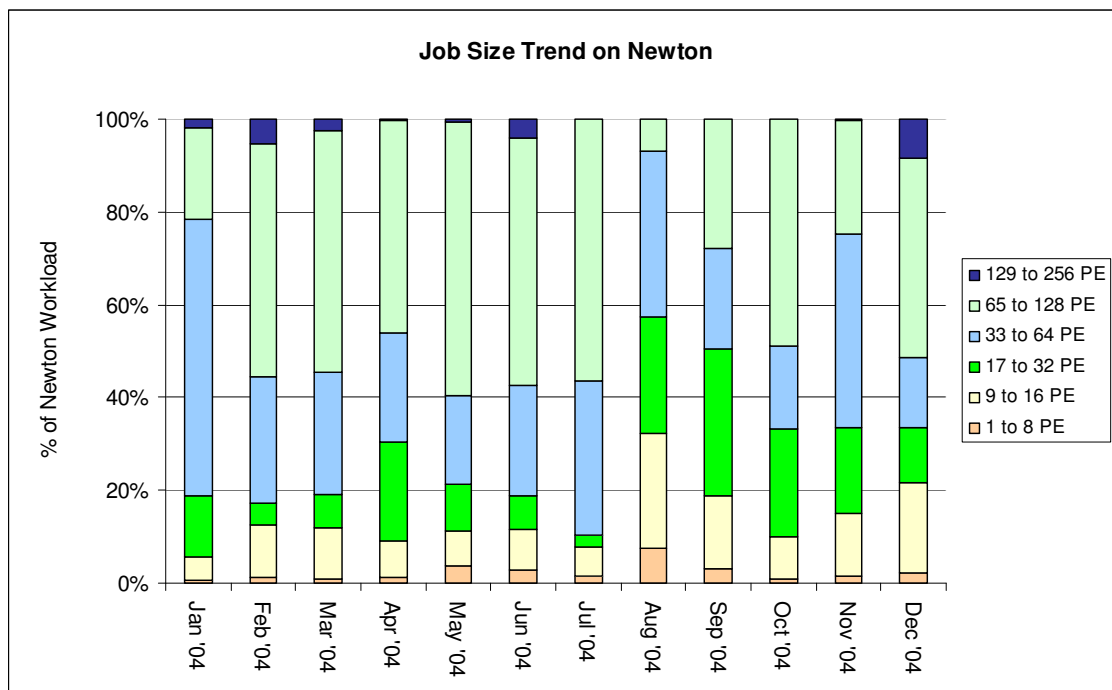
During the fourth quarter Newton's usage was reasonably spread across the machine.

2.2   System Usage Graphs

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

2.2.1   Baseline System

The graph below shows the Gflop Years utilisation on the CSAR systems by Research Council for the last 12 months.

MPP/SMP usage by Research Council
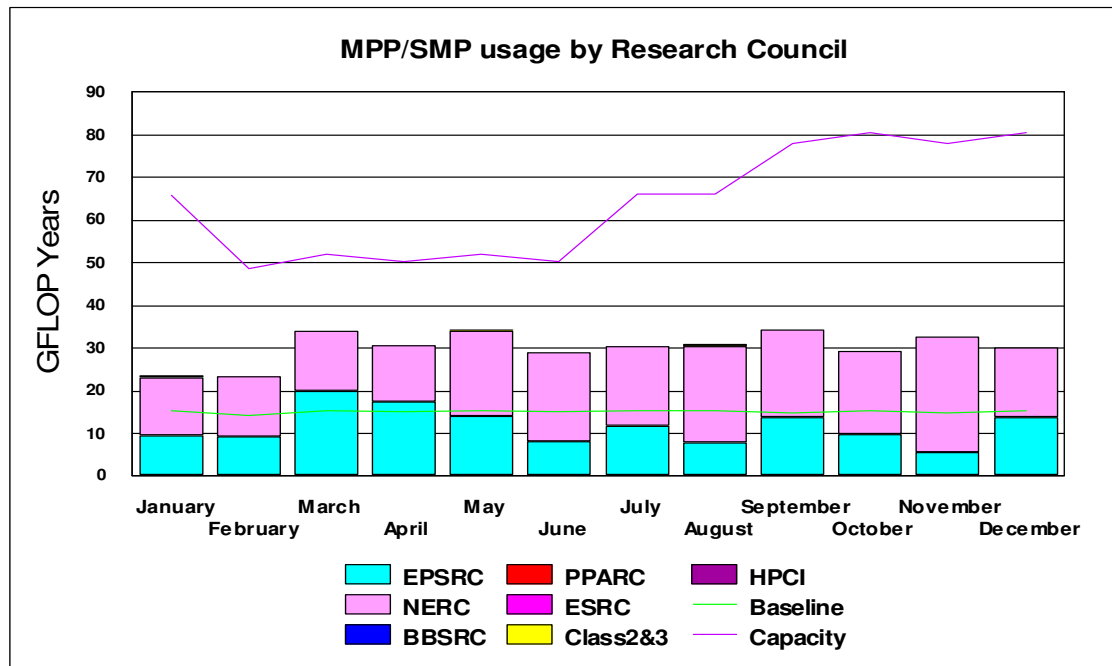
The graph below shows the same service utilisation by major system.
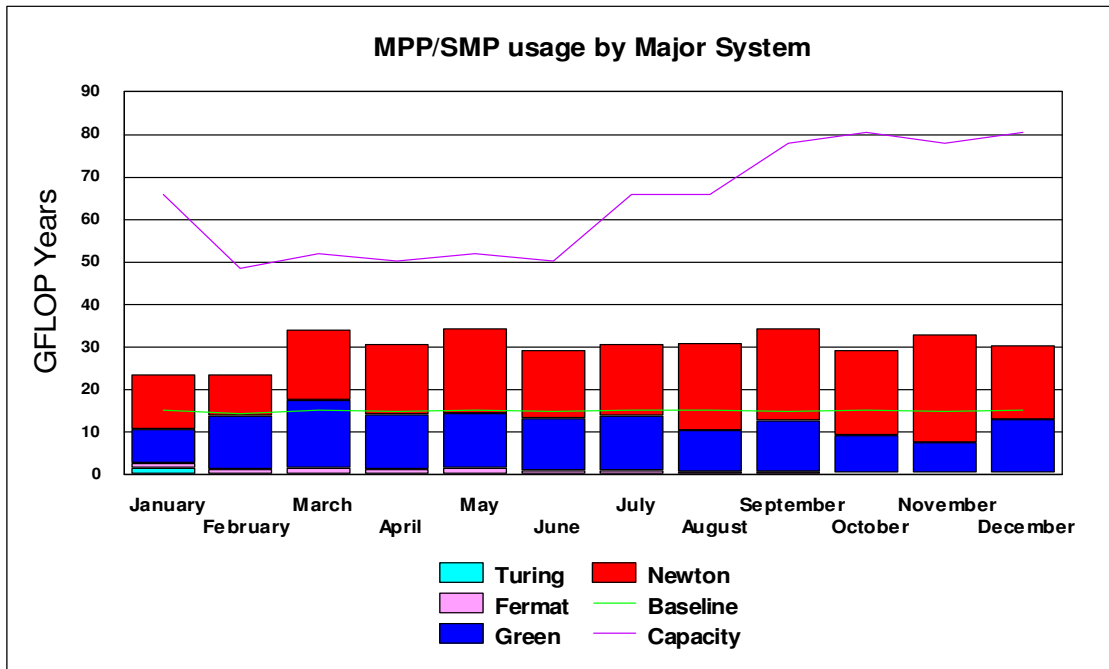
The next chart shows the historic interactive usage of the Origin 300 system Wren. Eight of the higher speed 500Mhz CPUs in Wren deliver the baseline capacity equivalent to that which was previously available on the Origin 3000 system Fermat for interactive usage.
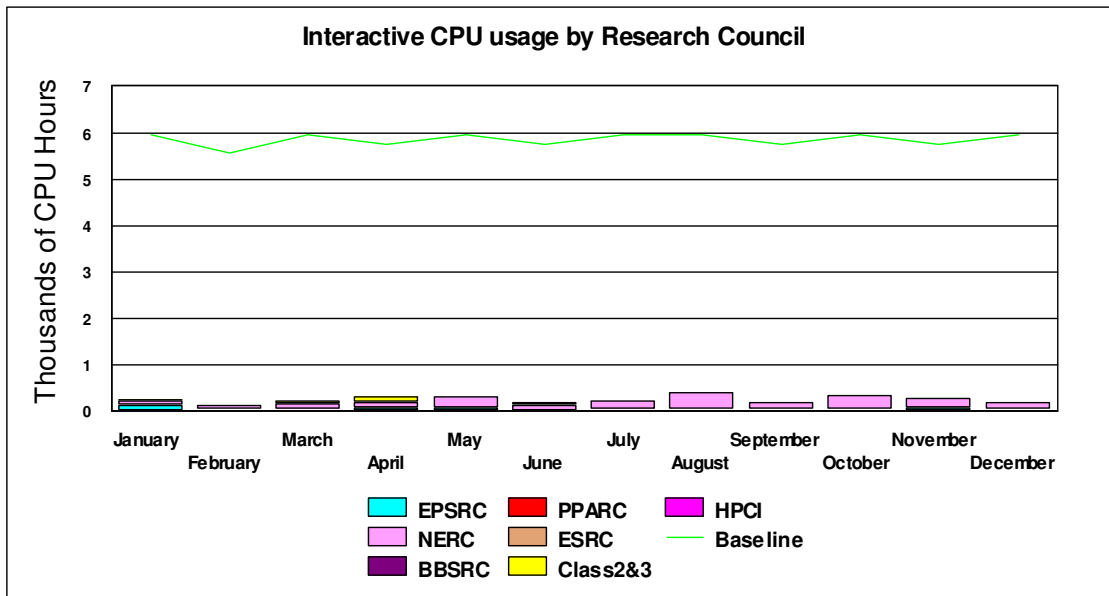
The following two charts detail the historic usage of the Origin 3000 system (Green) and the Altix 3700 system (Newton).
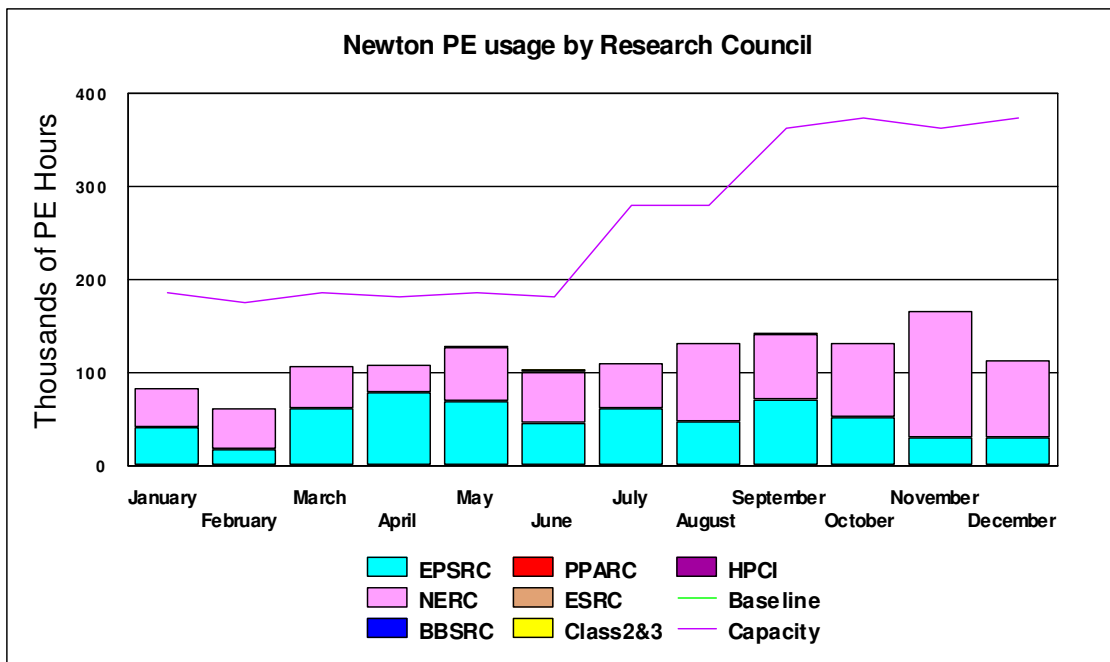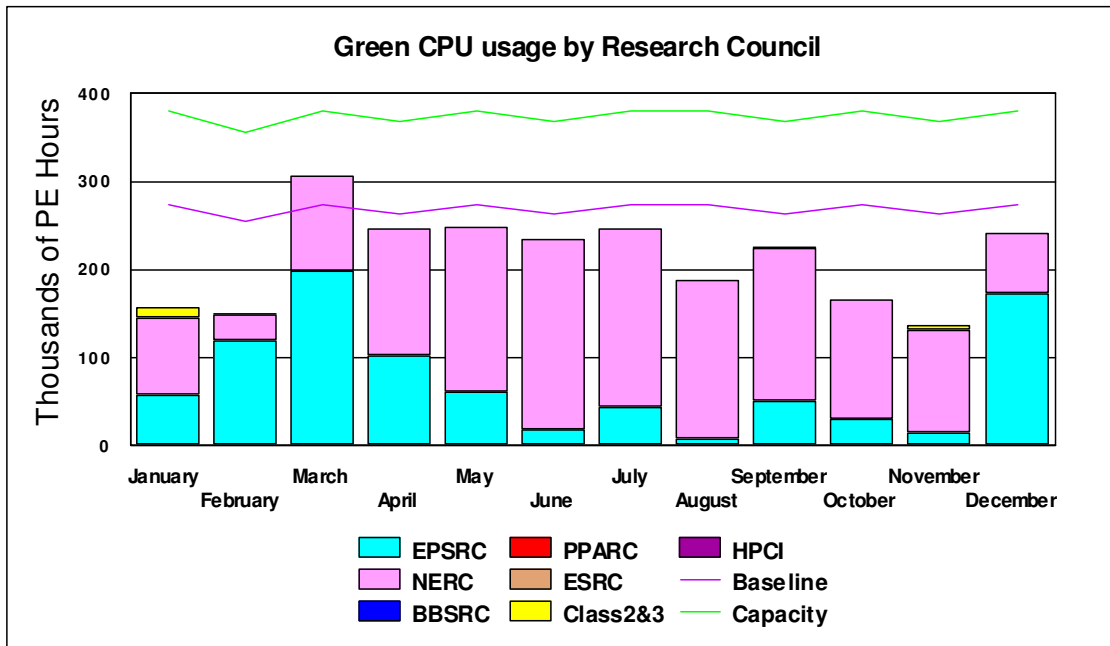
The next series of graphs illustrates the usage of the Medium Performance disk and HSM/tmp resources of the system.

MP Disk allocation by Research Council
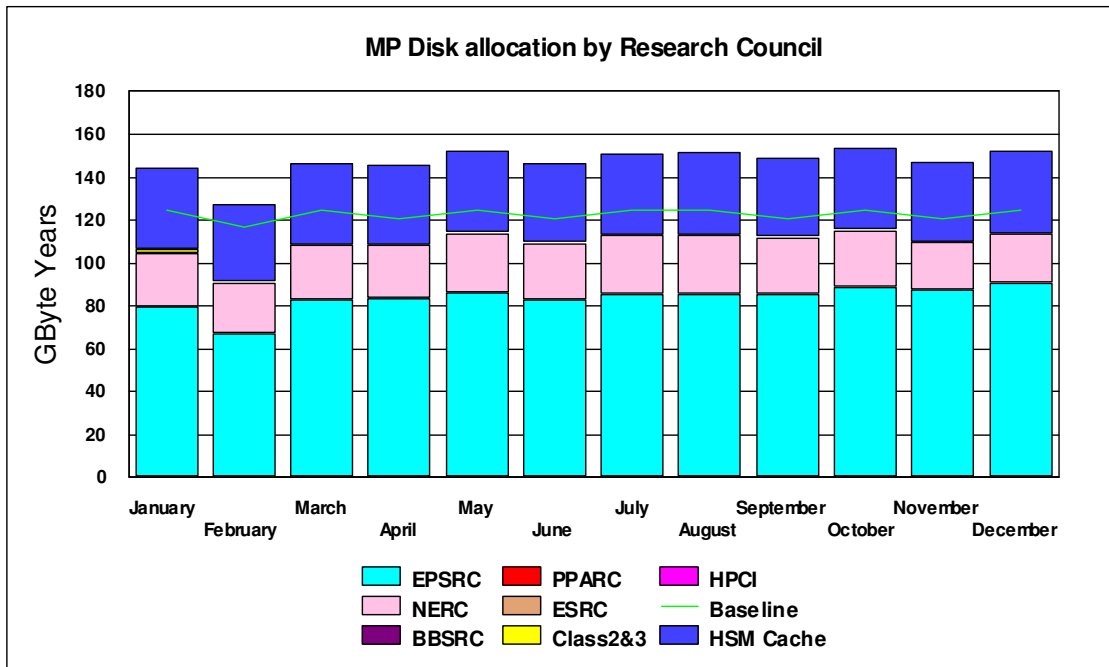
The above graph illustrates the historic allocation of the Medium Performance Disk on Fermat and the SAN.

The next graph shows the historic HSM usage by Research Council funded projects, which has exceeded the overall Baseline of 16 Terabytes, and now totals about 48 Terabytes.

HSM usage by Research Council
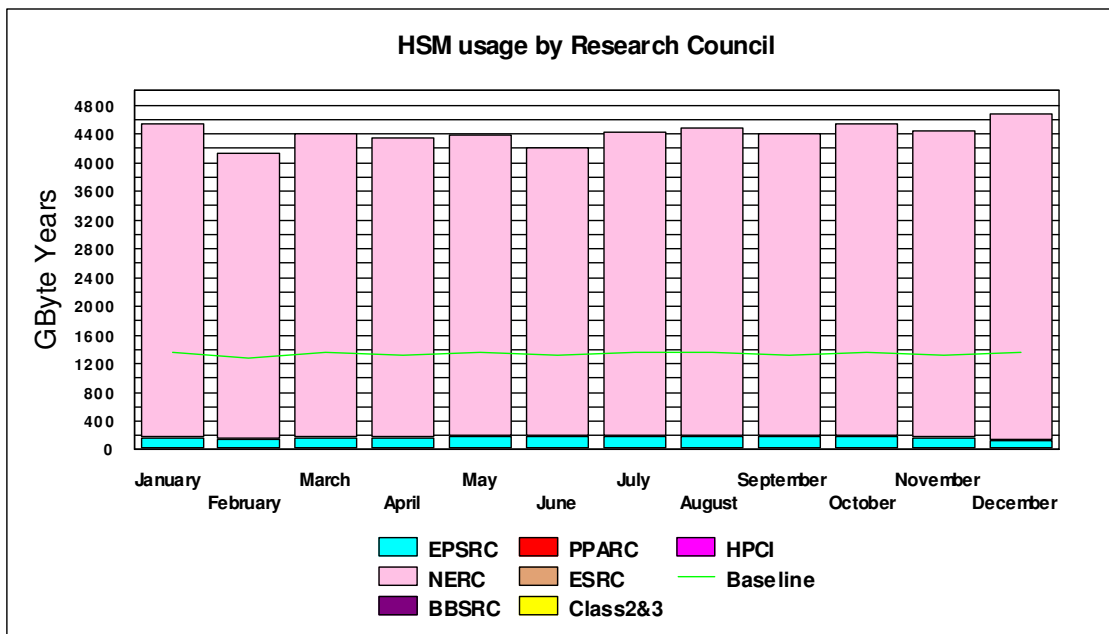
2.2.2   Guest System Usage

There is currently no Guest System usage.

2.3   Capability Incentives

Capability incentives were historically given on the T3E system Turing for jobs of 512 PEs and above. In July 2003 it was announced that discounts for capability jobs available on all CSAR systems had been approved to include the SGI Origin 3000 system Green and the SGI Altix 3700 system Newton.

These capability incentives were agreed with the Research Councils to encourage capability usage of the national supercomputers for greater scientific achievement, and offer the following discounts:

System	No of Processors	Discount
newton	192+ CPUs	15% discount
newton	128+ CPUs	10% discount
green	384+ CPUs	15% discount
green	256+ CPUs	10% discount

Discounts are given in the form of refunded Service Tokens.

Changes in usage patterns will be monitored and, subject to review, CfS reserve the right to change the incentives at any future date.

The following table displays the capability incentive discounts granted during the fourth quarter of this year.

Service Tokens Refunded: Quarter 4 2004 Usage							
System	Consortia						Total
	cse086	csn015	cse076	cse133	cs3025	csn066	
Green 256+ PEs	82.41	0.81					83.22
Green 384+ PEs							
Newton 128+ PEs			16.83	0.45	0.73	10.25	28.26
Newton 192+ PEs			0.01				0.01
Total Tokens							111.49

This is within the CfS Management Board's forecast.

2.4   Service Status, Issues and Plans

Status

The service has been reasonably utilised throughout the fourth quarter of 2004, with usage exceeding baseline.

There was a relatively balanced spread of work across all major systems throughout Quarter 4.

During the quarter, the original 4 x 64 processor Newton nodes were combined into one 256 processor Single System Image this month. Newton therefore now comprises of two 256 processor nodes, with one of the two nodes being made up of 128 x 1.3Ghz processors and 128 x 1.5Ghz processors.

Issues

There were some periods of system downtime during the middle of Quarter 4, due to a total building power outage at the University of Manchester and to some issues involving the SAN, however stability of the Altix system Newton was much improved during the final month of the quarter, owing to remedial patch work to the operating system carried out during this time..

Plans

It is planned to move both Newton nodes to a new building, potentially allowing for the two nodes to be combined into one 512 processor Single System Image if required. The move is expected to be carried out towards the end of January 2005, in a two-phase approach where one node is moved and brought back into production use before the other node is then moved. This is planned to minimise disruption to the user community and to ensure that a level of Altix service is maintained throughout the move.

3   Project Management, Documentation and User Feedback

This section covers aspects relating to the registration of projects and users, the management of projects and resources, topics associated with documentation and user feedback.

3.1   Project Applications

8 applications for new CSAR projects were received, requesting a total of 349,000 service tokens.

3.2   New Projects

7 new CSAR projects were started with 19,243 service tokens being awarded in total.

3.3   Finished Projects

2 projects finished

3.4   Queries

A total of 152 CSAR queries were dealt with:

- o   128 non-in-depth
- o   41 user registration and admin
- o   7 in-depth:

3.5   Service Quality Tokens

One user issued black marks and gold stars alternately over a short period reflecting levels of satisfaction with particular aspects of the service. This culminated in 3 gold stars. It is unusual for service quality tokens to be used in this way; such matters would normally be handled through the CSAR helpdesk.

3.6   Annual User Survey

The annual user survey took place in December 2004. There were 26 replies, 7 fewer than last year. In general the responses were very favourable, with 84% either satisfied or very satisfied with the overall service. There were, however, a small number of users who have found the Newton service less than satisfactory, primarily because of system instability and changes to the compilers. Both issues have been addressed and improvements made.

4   Scientific Application Support Services

4.1   Training and Education

- ▫ Introduction to HPC and the CSAR Service
- ▫ Shared Memory Parallelisation with OpenMP
- ▫ Introduction to MPI
- ▫ Advanced MPI
- ▫ MPI One-Sided communication and MPI-IO (New course)
- ▫ Origin 3000 Optimisation (Course significantly revised)
- ▫ Origin 3000 Parallel Scaling (Course significantly revised)
- ▫ Performance and Development Tools

4.2   Consortia Support/Software

The primary work has been in porting and optimising codes for the SGI Altix service, Newton, with additional testing on the 1.5GHz processors.

4.2.1 VASP

An optimised version of VASP 4.6.24, which includes bug fixes, has now been made available by SGI. This will be tested shortly.

4.2.2 PolComs

Additional optimisation work has been performed, with jobs using up to 128 processors. The scaling matches that of the original code and is roughly 10 times faster than the original code throughout. The 1.5GHz processors are roughly 1.2 times faster than the 1.3GHz. processors

4.2.3 H2MOL

Further modifications have been made, resulting in significant improvements in scaling on large numbers of processors.

4.2.4 NAMD

The latest version of NAMD, version 2.5, has been installed on the Origins and on Newton. Results of the ApoA1 benchmark on Newton have been sent to the developers for them to report.

4.2.5 DL_POLY

Version 3.02 has been installed on the Origins and on Newton.

4.2.6 FFTW

FFTW has been recompiled at version 8.1 of the compilers on Newton. This removes a problem encountered with CASTEP.

4.2.7 AMBER

Amber 7 has been rebuilt with version 8.1 of the compilers. The value of a parameter was increased to remove a limitation encountered by a user.

4.2.8 Tomcat

Further work is in progress in improving the scalability of the code.

4.2.9 ccSHT

The spherical harmonic transform library ccSHT was installed on Newton at the request of a user. Some modifications were made to the code to get the Fortran wrappers to work correctly.

4.2.10 Class 3 Project

Work has proceeded in the parallelisation of a code (LENS) on behalf of a Class 3 project. The code is currently working and scaling well, but with a couple of bugs currently under investigation.

4.2.11 Visualisation support

Visualisation work was performed for the Celebration of Engineering event in November. Subsequent discussions with some engineers have resulted in further requests for visualisation support. A site visit to Southampton involving visualisation training courses is being arranged for January 2005. One particularly interesting aspect to this is that the engineers are interested in stereo visualisation and that Manchester and Southampton both have stereo facilities linked to Access Grids.

4.2.12 New Users to HPC

Discussions have been held with PIs of three new projects awarded under the 2nd call for New Applications for HPC, all of whom requested significant CSAR support. The groups are still recruiting, so not yet ready to make substantial use of the service. As two groups are based in London, it is likely that tailored training courses will be delivered at one of the sites in London. For a fourth such project, in Supercomputer Datamining, Manchester is one of the partners and an appointment has now been made. Work will start in January 2005.

5   Collaboration and Conferences

5.1   MRCCS Projects

5.1.1 Advanced Virtual Prototyping Research Centre

The SCGlobal showcase entitled "Collaborative Finite Element Analysis" (Lee Margetts et al.) was presented via Access Grid at the SC 2004 conference in November 2004

Preparations are also underway to hold a workshop on virtual prototyping on 10th-11th March 2005.

Lee Margetts has submitted journal papers to *Transactions in Computer Graphics and Visualisation* and *Engineering Computations*, a conference paper to *NAFEMS World Congress* and an abstract for an invited keynote talk at the *ACME* conference.

5.1.2 NetSolve

NetSolve is an RPC based client/agent/server system that allows remote access of both hardware and software components. There are now developments to use Globus, which will help in the use of CSAR systems.

5.2   Events

Events attended include:

- The Eleventh ECMWF Workshop on the 'Use of High Performance Computing in Meteorology' on 25th-29th October 2004
- Supercomputing 2004, 8th-12th November 2004, Pittsburgh (see below)
- Celebration of Engineering, 17th November 2004, London
- Daresbury Machine Evaluation Workshop, December, Daresbury

The Celebration of Engineering event was a one day exhibition held as part of the International Review of Engineering in the UK. This is the 6th in a series of similar reviews, and the 2nd for engineering. It was co-ordinated by EPSRC and the Royal Academy of Engineering with Holly Benson Communications managing the exhibition itself at the ExCel Exhibition Centre in London.

A stand about 'HPC and Visualisation for Engineering' was displayed, in the theme 'Underpinning Technologies', by staff from Manchester Computing. The demonstrations, prepared and delivered by Joanna Leng and Lee Margetts, were displayed on a portable stereo projection facility hired from the University of Birmingham Information Services department.

The event was considered very successful, as noted particularly in the address by John O'Reilly of EPSRC.

6   Added Value Services

6.1   International Conferences

The main annual international conference of the Supercomputing community, 'Supercomputing 2004' or SC04 for short, was held this year in Pittsburgh in November. Manchester Computing, on behalf of the Supercomputing and other computational science activities of the University of Manchester as a whole (including the CSAR national HPC service), attended as usual in two forms: (i) we provided and manned a booth on the exhibition floor; (ii) we had a number of meetings with vendors and other parties, especially regarding product roadmaps and future trends in HPC etc. Note that in the context of this conference (and perhaps in the context of the United States in general), high end visualisation and grid technologies are considered to be part of Supercomputing – a close coupling that doesn't appear in the UK as strongly. It was also noted that the conference was as busy as ever, and it remains surprising, yet perhaps encouraging, that such a relatively small industry can sustain a conference of this size. The primary task of co-ordinating the exhibition presence and related issues was this year undertaken by Fiona Cook from the RSS/CSAR Frontline team. In addition to Fiona, the stand was manned in Pittsburgh by Kevin Roy, George Leaver, Rob Haines and Mike Robson. The exhibition presence this year went very well.

6.2   Visualisation

Progress continues in the collaboration between Access Grid technology and Manchester Visualisation Centre to create the first UK installation of a passive stereoscopic access grid node. Consisting of six Christie Digital LX32 projectors, an 8x2 metre real-laced passive stereoscopic surface, driven by three dedicated nVidia QuadroFX 3000G graphics cards. High-end scientific visualisation employing the standard commercial packages, such as AVS and Amira, will be available within the Access Grid.

6.3   Access Grid

There is increasing use of the Access Grid Support Centre (AGSC) hosted at Manchester. This is resulting generally in improvements in these facilities. More sites are obtaining the same software from the AGSC, simplifying the interaction between sites. For example, use of the Igpix software has helped when sharing presentations. Note that the Access Grid is used regularly for CSAR user meetings.