CSAR Service

Consolidated Management Report

1st Quarter 2004

Management Summary

This is the consolidated Management report for the first 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 429 to date.

The workload on both the Origin 3000 (Green) and the new Altix 3700 (Newton) has been fairly evenly spread across the mid- to high-end ranges of PEs during the first 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.

The newly introduced SGI Altix3700 system Newton has seen a good increase in uptake of use, and growth of usage continued throughout its first full quarter in production.

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

<u>Table 1</u> 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

	Performance Targets					
Service Quality Measure	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

<u>Table 2</u> gives actual performance information for the period. Overall, the CPARS Performance Achievement for the 1st quarter 2004 was satisfactory (see Table 3), i.e. Green measured against the CPARS performance targets.

	2003/4											
Service Quality Measure	April	Мау	June	July	Aug	Sept	Oct	Nov	Dec	Jan	Feb	March
HPC Services Availability												
Availability in Core Time (% of time)		97.66%	99.25%	98.83%	98.95%	96.62%	98.84%	98.95%	98.75%	97.49%	98.16%	98.51%
Availability out of Core Time (% of time)	99.81%	99.33%	99.9%	99.57%	100%	98.48%	99.28%	97.74%	98.3%	98.88%	97.9%	99.48%
Number of Failures in month	1	4		2	2	4	4	3	5	5	4	3
Mean Time between failures in 52 week rolling period (hours)	548	461	548	487	461	417	365	337	283	265	243	236
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
Non In-depth Queries - Max Time to resolve 95% of all queries		<1	<2	<1	<0.5	<5	<2	<1	<1	<2	<2	<2
Administrative Queries - Max Time to resolve 95% of all queries		<0.5	<0.5	<0.5	<1	<1	<1	<1	<1	<0.5	<0.5	<0.5
Help Desk Telephone - % of calls answered within 2 minutes		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
New User Registration Time (working days)		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
System Maintenance - no. of sessions taken per system in the mo		2	2	2	2	2	2	2	2	2	2	2

CSAR Service - Service Quality Report - Actual Performance Achievement

Notes:

<u>Table 2</u>

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)] + [Newton availability x 343/(40+23+343)] + [Newton availability x 343/(40+23+34

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

	2003/4											
Service Quality Measure	April	Мау	June	July	Aug	Sept	Oct	Nov	Dec	Jan	Feb	March
HPC Services Availability												
Availability in Core Time (% of time)		0.078	0	0.039	0.039	0.078	0.039	0.039	0.039	0.078	0.078	0.039
Availability out of Core Time (% of time)	-0.047	0	-0.047	-0.039	-0.047	0.078	-0.039	0.078	0.078	0	0.078	0
Number of Failures in month	-0.008	0.008	-0.008	0	0	0.008	0.008	0	0.0004	0.0004	0.008	0
Mean Time between failures in 52 week rolling period (hours)	-0.008	0	-0.008	0	0	0	0	0	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		-0.016	0	-0.016	-0.019	0.0312	0	-0.016	-0.016	0	0	0
Administrative Queries - Max Time to resolve 95% of all queries		-0.019	-0.019	-0.019	-0.016	-0.01551	-0.01551	-0.016	-0.016	-0.019	-0.019	-0.019
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
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
System Maintenance - no. of sessions taken per system in the mon		0	0	0	0	0	0	0	0	0	0	0
Monthly Total & averall Sonvice Quality Dating for each pariod		0.00	0.06	0.04	0.04	0.07	0.02	0.02	0.02	0.01	0.05	0.01
monuny rotar a overall service Quality Rating for each period:	-0.07	0.00	-0.06	-0.04	-0.04	0.07	-0.03	0.02	0.02	0.01	0.05	-0.01
Quarterly Service Credits:			-0.13]		-0.01]		0.02			0.05

Table 3

1.2 No. of Registered Users

The current position at the end of the quarter is that there are 429 registered users of the CSAR Service. The number of users saw a drop during October and November due to a number of projects that came to an end.



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 no black marks or gold stars had been allocated to the service.

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.



Usage of the SGI Altix 3700 system Newton is shown by Research Council in the above graph, from its introduction in October 2003.





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.



The above chart, and the one below, shows the wait time trend in hours on the Altix 3700 Newton.



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





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 1st quarter 2004.



On Green, the 65 to 128 PE range has seen the greatest percentage of workload during this quarter.





On Fermat the highest concentration of work was in the 17 to 32 PE range at 52%.

Newton's workload during its first full quarter in production has been spread fairly evenly across the system.



Usage on Green tended more to be in the mid-range of PEs during the 1st quarter.



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



During its first full quarter in production, 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.



The graph below shows the same service utilisation by major system. This quarter is the first without the T3E system Turing.



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



This 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 48 Terabytes.



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 aproved to include the SGI Origin 3000 system (Green) and the new 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 first quarter of this year.

Service Tokens Refunded: Quarter 1 2004 Usage											
System		Consortia									
System		cse085	cse086	csn003				TOLAI			
Green PEs	256+	33.8	14.6					48.4			
Green PEs	384+							0			
Newton PEs	128+	608.34		16.09				624.43			
Newton PEs	192+							0			
Total Tol	kens							672.83			

2.4 Service Status, Issues and Plans

Status

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

During the quarter there was a relatively balanced spread of work across all major systems.

The /hold facility was made accessible via the Storage Area Network (SAN) in January. This has meant that /hold is now available to users of the Altix system Newton, alongside users of the Origin systems who already had direct access to /hold.

Issues

There are no issues to report for this quarter.

Plans

Encouraging results of codes ported over to the SGI Altix 3700 system Newton have been seen, and work continues on porting/optimising further codes..

Both the Propack operating system of the Altix and the Irix operating system of the Origins are to be upgraded to a newer release during the second quarter 2004, offering benefits including greater stability for the Altix system Newton.

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

13 applications for new CSAR projects were received, requesting a total of 63354 service tokens.

3.2 New Projects

5 new CSAR projects were started with 44067 service tokens being awarded in total.

3.3 Finished Projects

5 projects finished

3.4 Virement from HPCX

There were three applications to transfer resources from HPCx to CSAR. All were successful.

3.5 Call for new applications to HPC

There was significant discussion with potential applicants, and project/code evaluation associated with the EPSRC call for new applications to HPC.

3.6 Project Management

An existing project was converted to one with subprojects in order to assist the PI in control resource utilization – the PI did not wish the alternative mechanism for such control by setting individual user allocations.

3.7 Capacity Planning

PIs were contacted, and other assessments made in order to improve the accuracy of the capacity plans, particularly with respect to the withdrawal of Turing from service.

3.8 Queries

A total of 232 CSAR queries were dealt with:

- o 141 non-in-depth
- o 78 user registration and admin
- o 13 in-depth

3.9 Service Quality Tokens

1 black mark was awarded in January because of the lack of a development queue on Newton. This had been discussed at the User Steering Group meeting in January, and was implemented shortly afterwards.

3.10 CSAR Focus

The Winter/Spring edition is close to publication.

3.11 CSAR Website

The new CSAR website is nearing completion and will be released in May 2004. Significant effort has been put into updating all sections of the website.

3.12 User Survey

The 2003 User Survey report has been produced and is available on the CSAR web pages.

3.13 User Steering Group

The 11th CSAR User Steering Group meeting took place in January. This was well attended, with much discussion about the service on Newton. The report from the User Liaison Forum chair (from Dr. Katherine Bouton, on behalf of Dr. Lois Steenman-Clark) summarized primary concerns about the Newton service, with particular reference to job scheduling. A number of steps were agreed, including the provision of a development queue and changes to the maximum time limits. (Details were given in the CSAR Bulletin and in the minutes of the meeting.).

4 Scientific Application Support Services

4.1 Training and Education

The following courses have been given:

- o Fortran 90
- o Introduction to MPI
- o Advanced MPI

4.2 Consortia Support/Software

Work has continued particularly on porting and optimising codes both for the new SGI Altix service, Newton, and for the SGI Origin systems. There continues to be great activity in this area

In general this has been very successful, with Newton performing at least 3 times faster than Green and 6 times faster then Turing in most cases. Additional details are given below.

4.2.1 Unified Model

Significant work has been performed with the Unified Model, on both the Origins and on Newton:

Version 4.5 has been built and tested with versions 7.1 and 8.0 of the compilers on Newton. The NCAS group is currently making extensive use with the 7.1 compiler. They are intending to use the 8.0 version once they have finished their own testing and updated all relevant scripts.

Version 5.3 (which is an interim implementation, prior to the major release, 5.5) has been built and tested on the Origins and on Newton with the 8.0 compiler.

Version 5.5 has been built and tested on the Origins and on Newton with the 8.0 compiler NCAS will start using this for production work once the Met Office has officially released this version, and after they have completed their own testing.

Implementation of the UM has resulted in the reporting of a significant number of compiler problems, particularly at 8.0. All of these have now been resolved – this has provided a thorough test for the compilers.

4.2.2 Castep

CSAR staff have been working in conjunction with Dr Keith Refson of RAL, one of the code developers, and bug fixes (in the code) have now resolved an outstanding problem that resulted in poor performance in certain circumstances. Significant improvements in performance have now been observed. This collaborative work is continuing.

4.2.3 NWChem

There had been performance issues in wall clock time with this code. The reasons have been identified and one solution has been tested successfully. An alternative approach in modifying the I/O in the code is now being pursued.

4.2.4 Molpro

Molpro was installed and tested. Results are being evaluated.

4.2.5 CPMD

There was a problem with running the CPMD code, but after extensive investigation by SGI, a fix was identified and the code now runs well.

4.2.6 Vasp

Version 4.4.3 has been built and successfully tested on Newton using version 7.1 of the compiler. Version 4.6.7 has been built with both 7.1 and 8.0 compilers. At 8.0, there are problems using full optimisation, but correct results obtained at -O2. However there is some concern about running across partitions on Newton. Both of these issues are being investigated.

4.2.7 NetCDF

This has been installed on Newton with versions 7.1 and 8.0 of the compilers.

4.2.8 Nav

The code 'Nav' has been ported to Newton with the 8.0 compiler.

4.2.9 Siesta

Some workarounds were found to compiler problems on Newton.

4.2.10 AVS

AVS/Express has now been set up for use via modules on the Origin systems.

4.2.11 Other third-party software

Gromacs -3.2.1, DL_POLY_3.01, hdf5, phdf5 and the Nag Fortran Library, Mark 20 have all been installed on Newton and on the Origins.

4.2.12 Other consortia porting/optimisation

Work continued on behalf of Dr Kai Luo and Dr Zhiwei Hu., and in the transfer of binary data from Turing with other users. Assistance was also given to a class 3 user when he extended his visit to Manchester Computing after attending some training courses.

4.2.13 Vampir, Totalview

Vampir, Vampirtrace and Totalview have been installed on Newton.

4.2.14 Visualisation support

Significant work was carried out on behalf of Dr Lionel Temmerman in producing high quality images for publications from data generated on the CSAR systems. The project, with Professor Michael Leschziner as the PI, studied the coupling of Turbulence models with LES strategies.

4.3 256 PE Single System Image

SGI provided access to a 512 PE system with a single system image for evaluation purposes. There are many advantages in providing a single system image for Newton (a single 256 PE partition instead of 4 64 PE partitions) This evaluation was to assess whether there are any code performance reasons for not doing so. A number of codes were run and results compared with production runs on Newton. In general, there were no code performance issues, although some specific points are still being investigated.

4.4 DDT

The DDT debugger provided by Streamline Computing has been evaluated on Newton and is currently being tested on the Origin systems. Streamline have made a number of changes and enhancements resulting from feedback from CSAR staff, and is now a stable and valuable tool, providing some functionality not available in Totalview. CSAR is now considering whether to recommend the purchase of DDT for the CSAR service.

4.5 Checkpointing on Green

Further testing of checkpointing on the Origin systems is taking place. If successful, this would significantly improve the scheduling capabilities, particularly large and/or development jobs.

5 Collaboration and Conferences

5.1 MRCCS Projects

5.1.1 Advanced Virtual Prototyping Research Centre

- o Working towards interactive stress visualisation.
- o Improved preconditioned conjugate gradient solver being implemented.
- o Assessing the largest problem sizes that can be tackled 'interactively' over a range of systems.
- o Further developments to the ParaFEM code, including the development of OpenMP alternatives.

5.1.2 GeoFEM collaboration

A pilot project has been set up for collaborative work with colleagues from Japan who were involved in developing the GeoFEM software as used for solid earth modelling in the Earth Simulator project.

5.1.3 The GeoSpace Visualisation Network

Following discussions at the Geo-visualisation meeting (see below), the 'GeoSpace Visualisation' Network was set up to provide a forum particularly for Geologists, Geophysicists, and Geotechnical Engineers interested in VR, and 3D visualisations - A web page has been set up at Manchester:

www.sve.man.ac.uk/Research/AtoZ/GeoSpace and Chris Harding at Iowa State University, US has set up a mailing list.

5.2 Events

- o Lee Margetts applied for and was awarded funding from the European Science Foundation to cover expenses and fees for the Geo-Visualisation 2004 conference. Joanna Leng co-authored paper
- o A seminar was given for ESNW on the 29th of January, entitled "Op3D-Grid, How One Medical Visualization Application was Adapted to Work With The Grid".
- o A demonstration on Op3D was given at the EPSRC ESNW review day on the 15th of March.
- o Attended the HPCx industry day.
- o A paper has been submitted to Vis2004 the most important visualization conference of the year.
- o Papers for the Eurographics UK conference have been reviewed. This year the papers will be published by IEEE
- CSAR staff are chairs of Special Interest Groups at both the Cray and SGI User Group meetings in May 2004. Proposed papers have been reviewed prior to the conferences, and papers are being prepared for the conference.

5.3 National Grid Service

Staff have been involved in setting up the National Grid Service, which starts service at the beginning of April 2004. This includes both a data node at Manchester and the CSAR service. This has included system management, running acceptance benchmarks and setting up the website.

6 Added Value Services

6.1 International Conferences

Preparations are being made for the International Supercomputing Conference at Heidelberg in June and for SC2004 at Pittsburgh in November, at both of which the University of Manchester will have exhibition stands.

Stephen Pickles will present a plenary talk at the ISC meeting about the Teragyroid experiments at SC2003, and receive the ISC award for the best paper in 'Integrated Data and Information Management'.

The University of Manchester has jointly submitted a tutorial proposal for SC2004 with collaborators from Japan involved in developing the GeoFEM software, used for the solid earth modeling on the Earth Simulator project.

6.2 Visits

There have been numerous visits from vendors and other HPC sites, including the Korean National HPC Centre and NASA Ames.