CSAR Service

Consolidated Management Report

2nd Quarter 2000

Management Summary

The system continues to be the flagship HPC facility for UK Academia and Industry, enabling World-Class research and development.

The number of users has grown to a total of 461 to date.

The upgraded Cray T3E (Turing) system has been highly utilised this quarter.

The STK silo upgrade for improvement of the HSM facilities is now in full production use.

CfS is currently 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 was good (see Table 3), i.e. Green measured against the CPARS performance targets.

| | 2000 | | | | | | | | | | | |
|--|--------|--------|---------|-------|--------|--------|--------|--------|--------|-------|-------|--------|
| Service Quality Measure | July | Aug | Sept | Oct | Oct | Dec | Jan | Feb | March | April | May | June |
| HPC Services Availability | | | | | | | | | | | | |
| Availability in Core Time (% of time) | 99.70% | 97.20% | 100.00% | 100% | 100% | 100% | 96.11% | 95.00% | 99.70% | 100% | 100% | 99.70% |
| Availability out of Core Time (% of time) | 99.40 | 98.41% | 99.40 | 100% | 100% | 99.70% | 98.52% | 100% | 99.50% | 99.5% | 99.40 | 99.40 |
| Number of Failures in month | 2 | 5 | 1 | 0 | 0 | 1 | 4 | 1 | 2 | 1 | 1 | 2 |
| Mean Time between failures in 52 week rolling period (hours) | 391 | 416 | 416 | 486 | 534 | 563 | 230 | 515 | 486 | 437 | 515 | 417 |
| Fujitsu Service Availability | | | | | | | | | | | | |
| Availability in Core Time (% of time) | N/A | N/A | N/A | N/A | 98.30% | 100% | 100% | 100% | 100% | 100% | 100% | 100% |
| Availability out of Core Time (% of time) | N/A | N/A | N/A | N/A | 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 | <2 | <2 | <2 | <3 | <2 | <1 | <1 | <1 | <2 | <1 | <2 | <1 |
| Administrative Queries - Max Time to resolve 95% of all queries | <1 | <1 | <1 | <2 | <1 | <0.5 | <0.5 | <1 | <2 | <1 | <2 | <0.5 |
| 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 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 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 mon | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 2 |

CSAR Service - Service Quality Report - Actual Performance Achievement

Notes:

Table 2

- 1. HPC Services Availability has been calculated using the following formulae, based on the relative NPB performance of Turing and Fermat at installation: [Turing availability x 122 / (122 + 3.5)] + [Fermat availability x 3.5 / (122 + 3.5)]
- 2. Mean Time Between Failures for Service Credits is formally calculated from Go-Live Date.

<u>Table 3</u> 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

| | 2000 | | | | | | | | | | | |
|--|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Service Quality Measure | July | Aug | Sept | Oct | Nov | Dec | Jan | Feb | March | April | May | June |
| HPC Services Availability | | | | | | | | | | | | |
| Availability in Core Time (% of time) | -0.039 | 0.078 | -0.058 | -0.058 | -0.058 | -0.058 | 0.195 | 0.195 | -0.039 | -0.058 | -0.058 | -0.039 |
| Availability out of Core Time (% of time) | 0 | 0.039 | 0 | -0.047 | -0.047 | -0.039 | 0 | -0.047 | -0.039 | -0.039 | 0 | 0 |
| Number of Failures in month | 0 | 0.016 | -0.008 | -0.009 | -0.009 | -0.008 | 0.008 | -0.008 | 0 | -0.008 | -0.008 | 0 |
| Mean Time between failures in 52 week rolling period (hours) | 0 | 0.016 | 0 | 0 | -0.008 | -0.008 | 0.008 | -0.008 | 0 | 0 | -0.008 | 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 | 0 | 0 | 0.016 | 0 | -0.016 | -0.016 | -0.016 | 0 | -0.016 | 0 | -0.016 |
| Administrative Queries - Max Time to resolve 95% of all queries | -0.016 | -0.016 | -0.016 | 0 | -0.016 | -0.019 | -0.019 | -0.016 | 0 | -0.016 | 0 | -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 | -0.004 |
| Others | | | | | | | | | | | | |
| Normal Media Exchange Requests - average response time | N/A |
| New User Registration Time (working days) | 0 | 0 | 0 | -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 mon | 0 | -0.003 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -0.003 | -0.003 | 0 |
| Monthly Total & overall Service Quality Rating for each period: | -0.04 | 0.08 | -0.05 | -0.07 | -0.09 | -0.09 | 0.07 | 0.03 | -0.06 | -0.09 | -0.06 | -0.06 |
| Quarterly Service Credits: | | | -0.01 | | | -0.25 | l | | -0.06 | I | | -0.21 |

Table 3

1.2 No. of Registered Users

The current position at the end of the quarter is that there are 461 registered users of the CSAR Service.

It can be seen from the chart below that the number of users continues to grow steadily.



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.

There are, at the end of the quarter, four Gold Stars allocated to the service.

| No of Stars or Marks | Consortia | Date Allocated | Reason Given |
|-------------------------|-----------|-------------------|----------------------------|
| 4 Gold Stars | CSN003 | 14/06/00 | Applications Support work. |

SUMMARY OF SERVICE QUALITY TOKEN USAGE

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) MPP (T3E) Usage by month, showing usage each month of CPU (T3E PE Elapsed Hours), split by Research Council and giving the equivalent GFLOP-Years as per NPB. The Baseline Capacity is shown by an overlaid horizontal line.
- 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.

2.1 Service Usage Charts

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





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

Origin2000 CPU usage is shown by Research Council during the last 12 months of service is shown in the above chart.



The chart above shows the average wait time trend over the last 12 months. Despite the major upgrade to Turing (adding 26% to the capacity), wait times are now however growing due to the heavy workload.



It can be seen from the above graph that enhancements to the scheduling on Turing did reduce the average wait times but attention must be paid to ensure sufficient head room exists in the system to prevent wait times from rising. It is intended that the provision of the planned SGI IA-64 systems will assist in better meeting the growth in user demands.





The trend on job size is upwards.

2.2 System Usage Graphs

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

2.2.1 Baseline System

The graph below shows the PE hour's utilisation on Turing by Research Council from July 1999.



The graph below shows the historic CPU usage on Fermat by Research Council from July 1999.



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.



The graph above illustrates the historic allocation of the Medium Performance Disk on Fermat. From July 2000, 200 Gbytes will be used as a data cache for the enhanced HSM system.

The graph below shows the historic HSM usage by Research Council funded projects. The primary usage is for NERC.



2.2.2 Fujitsu System Usage Graph



The above graph shows the current CPU usage on the Fujitsu VPP 300 NERC system based at the University of Manchester. The Fujitsu usage exceeded the baseline usage in May for the first time since last November.

2.2.3 Guest System Usage Graphs

There are currently no Guest systems available to the CSAR service, but there are plans to add Compaq, HP and NEC systems from around August 2000

2.3 Service Status, Issues and Plans

Status

The service has run above baseline since the 200 PE upgrade was carried out in March.

The upgrade of the silo is now in use on the production system.

During the Quarter, 64% of the jobs run on Turing were larger than 33 PEs in size.

Issues

Wait times are growing with increasing demands for the services.

Plans

Plans are underway to integrate the ASCI prototype system (Fourier) due to arrive in August.

Appendix 1 Contains details of the current capacity planning information and projections.

3 Collaboration and Conferences

3.1 UKHEC Collaboration

3.1.1 Visualization case studies

The first of three visualization case studies for UKHEC has utilized data from Huw Davies of the Terra group who are running simulations of the earth's mantle to compare with geophysical seismic data. This work has produced a successful visualization of a tomography data set with a complex structure and very large volume. Novel techniques for coping with the spherical geometry and very large range of pressure and temperature variations have been developed. This work has been reported in the Spring UKHEC newsletter and in CSAR Focus No. 5. A paper describing the work has been given at the Cray User Group (CUG) summit (May 22-26). A paper has also been submitted to the SGI User Group in Krakow (October 11-14 2000). This work benefited greatly from the loan of an SGI Octane workstation under the CfS graphics workstation loan scheme.

3.1.2 UKHEC Seminar and Workshop on Grid Computing

This workshop was held on June 21-22 at Daresbury as a joint collaboration between Daresbury High Performance Computing Group and MRCCS. There were talks on GRID computing given by experts from the US, Europe and Japan. On the second day there was a joint Science Applications Support Services presentation by MRCCS and HLRS (Stuttgart) of the methods used in the global metacomputing experiment which won an award at SC99. This also included a hands-on session to allow participants to work with a GRIDenabled MPI library (PACX-MPI). A paper based on this work was awarded the Best Paper award at HPCN2000 and the work was also presented at the CUG.

3.1.3 UKHEC Report on Grid Computing for the UK

MRCCS collated a report on the relevance of GRID computing for UK Science in collaboration with Daresbury, EPCC and RAL. As part of this report experiments were set up between all four sites using the Globus toolkit to launch jobs and run between sites. Of particular relevance to CSAR were creation of a graphical front-end to Globus to allow jobs to be submitted to the T3E machines at CSAR and EPCC. A paper describing this and other GRID initiatives at CSAR has been submitted to the GRID2000 conference this December.

3.2 GRID Developments

Mr W T Hewitt attended the 3rd Grid Forum in San Diego. He established contact with a number of groups, most especially Dr C Catlett at the Argonne National Lab. He is responsible for a proposal to NSF to establish a Beta Grid. We are discussing ways in which CfS could join this project should it receive funding.

A Manchester Grid has been established. Both Globus and Unicore have been installed on several machines at Manchester (both CfS and University of Manchester) and experiments are underway.

A videoconference, led by CfS, was held. RAL, DL, EPCC, Manchester and CfS were represented and we agreed to a number of single site, dual site and triple site experiments. The aim is to produce a report for EPSRC for the 24th July, CfS Management Board. We will try to produce a draft version a month before that. The videoconference meeting also noted that UKHEC (DL, EPCC, MRCCS) had already produced a report (yet to be published) describing GRID and Metacomputing.

3.3 Collaboration with 'HPCI Centres'

MRCCS is one of the partners in the UKHEC consortium which provides support and information of current developments in high-end computing. This has enabled CSAR to continue its fruitful collaboration with the former HPCI centres. One very useful result has been the exchange of information/expertise with Daresbury over matters of cluster computing and the newly emerging GRID technology.

Speakers from both EPCC and Daresbury gave seminars in the MRCCS series and this allowed valuable informal contact between the major HPC centres to maximise expertise and avoid wasteful duplication of effort.

3.4 Conferences and Workshops

The following conferences/workshops have been attended.

A presentation was given at the 8th conference of the Association of Computational Mechanics in Engineering (ACME), University of Greenwich, April 16th-19th.

The Grid Forum, San Diego, April

EGRID workshop, Poznan, Poland, April

An award of the 'Best Conference Paper' was made for the presentation by Costen at the 8th conference on High Performance Computing and Networking, Europe in Amsterdam, 10th-12th May.

High Performance Computational Modelling Facility Open Day, University of Leeds, May 10th.

Four presentations were given at the Cray User Group (CUG) meeting in Noordwijk, The Netherlands, May 22nd-26th. This covered service aspects, visualization, metacomputing and OpenMP programming.

The 2nd European Advanced Computing Technology Centre (ACTC – part of the IBM Advanced Computing Technology Centre) workshop in Paris, 24th-26th May

Presentations were made at the METODIS and Metacomputing Workshops at HLRS in the University of Stuttgart, June 5^{th} - 7^{th} .

MRCCS was one of the co-organisers of the Grid Workshop, held at Daresbury Laboratories, 21st-22nd June.

More presentations were given at the Virtual Tissue Engineering workshop, University of Leeds, June 21st-22nd. This involved the application of numerical and engineering analyses with visualization, to tissue behaviour, with particular reference to the heart.

4 User Registration and Project Management Services

This section covers aspects relating to the registration of projects and users, and the management of projects and resources.

4.1 Quarterly usage reports by email

The second of the quarterly emails providing a summary of actual and planned usage will be sent to PIs during July. These summaries will cover the six month period from January to June 2000. The first of these emails sent

out in April appears to have been of use to a number of PIs in bringing their attention to recent usage levels. However, we have yet to observe and noticeable improvement in the accuracy of projects' capacity plans.

4.2 Conditions of use

It was reported in the last quarterly report that the conditions of use of the CSAR systems was to be revised imminently in order to comply with current UK Department of Trade and Industry regulations on access to HPC systems. All new users of the service are now required to accept these conditions when they register, and all existing users were asked by email on 9th May to confirm that they agree to the conditions. Users were pre-warned of the request by Professor Taylor, Chair of the User Steering group.

To date we have had responses from 54% of the 440 existing registered Class 1/2/3 users, all of them accepting the conditions. Just one user queried the conditions in relation to possible third-party use of research subsequently put into the public domain. Clearly users cannot take responsibility for this, and thus there was no reason for him not to accept the conditions.

We are maintaining an email list of those users who have yet to respond, and we will use this list to send a reminder in the near future. It is expected that more than one reminder will be required in order to obtain responses from all users.

5 Added Value Services

5.1 'ASCI' Prototyping Facility

EPSRC has approved the proposals for this facility. CfS is now drawing up more detailed plans of the installation and development of this service.

5.2 Visualization Software

The 'Visualization in Parallel' package, VIPAR, developed by MVC is now being ported to the SGI Origin 2000, using the latest versions of MPI and AVS Express in order to address a request from one of the CSAR consortia.

5.3 Joint Projects

The first phase of the development of AVS Express multi-pipe edition (which uses the SGI multi-pipe graphics library) has now been completed. Further funding has now been obtained and phase II is underway. Improvements and bug fixes to the software are being incorporated.

5.4 6th SGI/Cray MPP Workshop, September 7th-8th

Organisation of the workshop is progressing well. About 27 abstracts have been received and approved by the programme committee. A few more are still expected.

5.5 Summer School 2000, September 4th-15th

This is also progressing well. About 15 people have so far registered.

5.6 International Conferences

Eurographics 2001: 3 keynote speakers have been agreed. Posters have been prepared. Europar 2001: The Programme Committee is being finalised.

For both conferences, the Call For Papers is scheduled to be advertised in August.

5.7 Seminars

The second series of weekly seminars for HPC and visualization has now completed. Occasional seminars are being held during the summer – the first one, given by Tom Goodale on the Cactus Computational Toolkit project, generated much interest. Preparations are now being made for the series starting in October 2000.

5.8 European Projects

MRCCS is the UK representative among the major European sites involved in the EUROGRID project, which will link supercomputer centres in the UK, Germany, France, Poland and Norway and includes partners from industry and governmental organisations. This project will lay the basis for a European Grid and will produce middleware of importance for the development of E-Science. MRCCS is particularly concerned with the development of a resource broker which will allow scientific groups to seek out the resources that they require. MRCCS is also involved the production of middleware to facilitate the processing of data from experimental and observational facilities over the European GRID. An important aspect of a European GRID is that it links with global developments in GRID computing and MRCCS has active links with the major GRID developers in the US and in Japan. This global work will be presented at the forthcoming iGRID meeting in the US (July 19/20) and at SC2000 in Dallas this November.

5.9 Summer Students

The summer student program for 2000 has now started. The projects cover a wide variety of topics involving the web, visualization, meta-computing and mixed-memory parallel programming.

6 Science Application Support Services

6.1 Consortia Support

The parallelisation/optimisation of CASTEP on behalf of the UKCP consortium has reached a significant milestone, with the release of version 4.2 on CD to relevant CSAR users. The value of this work has been emphasised not only by the UKCP consortium themselves, but also by Molecular Simulations Inc. (MSI), who distribute the code worldwide. In a recent press release, they stated 'CASTEP,..., can now run between 50 and 100 times faster than before on designated computer architectures. This makes it possible to model larger molecular and solid-state systems,...'

The parallelisation of a serial lattice code for Professor Coveney at QMW (CSE030) is also virtually complete, with the group expecting to make significant use of this code for some systematic large simulations now planned. This work involved parallelising a code completely from scratch and was funded by support tokens. The exercise has been very valuable in developing the CSAR team's ability to negotiate large-scale support via the tokens scheme and have shown that this scheme can provide a way in which users can evaluate the progress of support effort and have a set of objectives by which this progress can be judged.

The success of both of these projects is indicated by the fact that both groups have now requested CSAR support for quite separate projects – the MPP development of another computational package, CRYSTAL, and the development of visualization tools.

The visualisation work for the Terra group has made substantial progress and the Terra group has commented very favourably on the results. This work is being disseminated to the UK community via a case-study report for UKHEC and forms the centrepiece of an article on visualisation in the UKHEC newsletter.

Work on coupling ocean-atmosphere models has been made available to the Occam group who are evaluating its potential for production use. International links with other groups running coupled models have been made via a visit and presentation to CERFACS and this expertise is available to CSAR users.

Other support has included some I/O optimisation, resulting in significant improvements, parallel debugging and some additional cache optimisation.

The offer of a free evaluation of applications by the Applications/Optimisation team has been taken up by several groups and relevant results from this exercise forms the basis of articles to the UKHEC newsletter and will feature in the next edition of CSAR focus.

The experience gained from support work is being used to advise the Research Councils on the support needs of new project applications. It is clear that for the majority of projects, sufficient support tokens need to be built into the initial application and that where this has been done, projects have reaped considerable benefit.

6.2 Training and Education

The courses for the second semester of the year 1999/2000 have now finished. A wide range of courses has been offered, but there is still concern over the attendance. The exception to this was the latest MPI courses which were given outside normal term times and were very well attended. The timing is thought to be relevant, so more effort will be made to schedule courses at such times in the future.

The course schedule for the first semester of 2000/2001 is now being drawn up. Some courses will be dropped in order to give more emphasis to those most relevant to the CSAR community. Development of new IA64 based courses will start once access to such systems and staff training has taken place. It is expected that the first such courses to be scheduled will be in the second semester of 2000/2001.

6.3 Service Developments

The Summer 2000 edition of CSAR Focus has been published.

There have been a number of updates to the applications software:

- Gaussian 98 has been installed;
- DL_POLY has been updated to the latest release;
- another computational chemistry package, NWChem, has been installed;
- The Nag Fortran Library has been updated to Mark 19.
- A 2D graphics library, PGPLOT has been installed.
- NetCDF version 3.3 has been installed on fuji

Approval has been sought for the purchase of the performance analysis tool VAMPIR and the parallel debugger Totalview on fermat.

Work has proceeded on provision of the secure shell on all CSAR facilities and this service should be available shortly. It will be announced via the usual channels.

CSAR applications have worked with systems managers at CSC to investigate and improve the performance of applications running on command PEs. This work has resulted in recommendations which are currently being tested prior to implementation and announcement.

Appendix 1

The capacity planning information, illustrated in the next graph, shows users projected demands for PE hours on the primary engine within the CSAR Service, the 776 PE T3E 1200E (Turing).

It can be see from the graph that user demands for PE hours in this 6 month period are in excess of one thousand PEs, however historically the user community have underused against their actual planned usage. There is a risk, however that high actual demand will result in long queue times.

The upgrade to Turing that was carried out in the first half of the current year has provided considerable additional capacity which the users are using very effectively. Usage was 47.5% over Baseline in June, and 13% below the current capacity.

The capacity planning information for 2001/2002 does not give a true picture, as the forecast future demand from current/new projects is based on incomplete records of likely Grant and resource allocations.

The graph does show a shortfall in the current capacity against demand, but it is difficult to justify expenditure on additional existing technology to bridge this gap. The CfS plan is for the additional capacity to be provided by a move to the newer technologies, such as the SGI IA-64 ASCI system, Fourier, also the addition of new Guest systems. It is intended that this will provide sufficient headroom in the services to meet any demands over and above the current capacity.

The SGI SN-IA system, planned for the Technology Refresh by end 2001, will at least meet the increased Baseline requirement – and will be scaled to meet capacity demands as then planned.

