The Australian National University

Supercomputer Facility

Annual Report 1999-2001

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The cover image depicts a network model for simulating fluid flow through porous rock. The patterns of cavities and connecting tunnels are abstracted from rock samples via 3D computerised tomography. Using a process of computed percolation to invade this model, the path of the fluid through the network can be visualized.

This research is by Dr Mark Knackstedt and Dr Adrian Sheppard of the Department of Applied Mathematics, RSPhysSE and Dr Rob Sok of the Petroleum Engineering Department, University of NSW with visualization by Stuart Ramsden, ANUSF VizLab. Cover design by Drew Whitehouse, ANUSF VizLab.

Contents

Abbreviations Used

Schools

ACAT	Australian Centre for the Arts & Technology
ANUSF	Australian National University Supercomputer Facility
CMA	Centre for Mathematics and its Applications
CRES	Centre for Resource & Environmental Studies
CSL	Computer Sciences Laboratory
DCS	Department of Computer Science
FEIT	Faculty of Engineering and Information Technology
JCSMR	John Curtin School of Medical Research
MSSSO	Mount Stromlo & Siding Spring Observatories
RSAA	Research School of Astronomy and Astrophysics
RSBS	Research School of Biological Sciences
RSC	Research School of Chemistry
RSISE	Research School of Information Sciences and Engineering
RSPAS	Research School of Pacific and Asian Studies
RSPhysSE	Research School of Physical Sciences and Engineering
SMS	School of Mathematical Sciences

Other

AARNet	Australian Academic Research Network
ACSF	Australian Cooperative Supercomputer Facility
ANZIAM	Australian and New Zealand Industrial Applied Mathematics
APAC	Australian Partnership for Advanced Computing
DETYA	Department of Education, Training and Youth Affairs
FECIT	Fujitsu European Centre of Information Technology
HPCAC	High Performance Computing Advisory Committee
HPCLab	High Performance Computing Laboratory
MAS	Merit Allocation Scheme for APAC National Facility
MDSS	Mass Data Storage System
PARSA	Postgraduate and Research Students Association
PI	Principal Investigator
RIBG	Research Infrastructure Bulk Grant
RIEF	Research Infrastructure Equipment and Facilities
STAC	Supercomputer Time Allocation Committee
VizLab	ANUSF Visualization Laboratory
VR	Virtual Reality
VE	Virtual Environments

Role

The role of the ANU Supercomputer Facility (ANUSF) is to support computational science, engineering and other research fields through the provision of both high performance computing (HPC) infrastructure and expertise. The infrastructure is composed of four basic elements – computational systems, visualization (including virtual environments), networks and systems for handling massive amounts of data. All elements except networking are the direct responsibility of the Supercomputer Facility.

Expertise is provided at all levels, from basic operational support to algorithm development and implementation to collaboration in research projects. The Facility is also involved in industrial R&D projects and Computational Science and Engineering education programs with the Department of Computer Science, FEIT.

Since mid-1999, the ANUSF has also been responsible for fulfilling the University's commitments to support the National Facility of the Australian Partnership for Advanced Computing (APAC).

A detailed ANUSF Annual Report was not published for 1999-2000 in the light of possible structural re-organizations of high performance computing within the ANU resulting from the formation of APAC. Therefore this report, while focussing on 2001, includes some material relating to those earlier years.

Highlights of 1999-2001

Head's Overview

Since the publication of the last ANUSF Annual Report, the most exciting development has been the establishment of the APAC National Facility located at the ANU and supported by ANUSF staff. This facility, ranking in the top 31 worldwide, presents a great opportunity for Australian researchers in general and ANU researchers in particular.

The APAC-supported Centres of Expertise at ANU will further strengthen the University's programs involving the application of high performance computing systems. With the APAC Computing Tools and Techniques Centre of Expertise led by National Facility staff, and the forthcoming GrangeNet projects, there is a tremendous opportunity for the ANU to take a national leadership role in high performance computing and communications.

Since 1998, the High Performance Computing Advisory Committee has recommended the establishment of an ANU Computational Centre, incorporating the ANUSF, so as to take full advantage of these opportunities and to maximise the return on the University's long-term investment in HPC. Unfortunately it has not yet been possible to achieve this goal.

The establishment of the APAC National Facility has created an immense workload for ANUSF staff in recent years. I would like to thank the ANUSF staff for their tireless work to ensure the smooth operation of the facility and all processes concerned with administering and supporting the Facility and its users.

Bob Gingold

Head, ANUSF

National High Performance Computing and Communications Program Commenced

The Australian Partnership for Advanced Computing, APAC, was launched by Ms Trish Worth, MP, Parliamentary Secretary to the Minister for Education, Training and Youth Affairs in a ceremony at Parliament House in October 1999. APAC's goal is to enhance Australia's international position in high performance computing, placing the nation in the top ten countries in the application and development of this technology. The national partnership was seeded with an allocation of $19.5M from the Department of Education, Training and Youth Affairs. The overall APAC program and Partner activities involve investments of the order of $80M over three years by Partners in five states, the ANU and the CSIRO.

The ANU is the host organization for this national partnership and is hosting APAC's National Facility which consists of a peak computer system linked to ANU's massive data storage system and visualization laboratory. Under an agreement with APAC, the ANU is providing accommodation for the peak computer with staff support provided through ANUSF.

The National Facility service commenced on 30 April 2001 and was officially opened by Dr David Kemp, MP, Minister for Education, Training and Youth Affairs on 18 May 2001.

As well as improving the high performance computing infrastructure available to researchers, APAC is conducting programs centred on its Partners in the areas of education, research and industrial diffusion of high performance computing technology. In 2000, APAC approved three Centres of Expertise programs at the ANU (Computational Chemistry and Biology, Data Mining and Mesoscale Physics) as well as an education program in Computational Science and Engineering. The National Facility staff also took responsibility for conducting a Centre of Expertise in Computing Tools and Technology.

The National Facility has been heavily used, attracting 143 projects under a national Merit Allocation Scheme and through Partner shares. In the first 8 months of operation a further 84 'start-up' projects brought the total number of researchers associated with projects to 531 with nearly 500 having user accounts. Requests for resources under the Merit Allocation Scheme made late in 2001 exceeded that available by more than a factor of three. ANUSF staff have been active in presenting courses on using the National Facility in every state (except SA which had yet to join APAC). These 'hands-on' courses had been presented to almost 200 researchers and students by the end of 2001.

In May 2001, a consortium led by AARNet and APAC was allocated $14M for GrangeNet (Grid and Next Generation Network) under the Federal Governments BITS Advanced Network Program. This network will connect several of the APAC Partners, including the ANU and the National Facility, with a high-speed broadband network. The ANU will be involved in projects in Advanced Communication Technologies and in Grid Services commencing in 2002.

Visualisation Laboratory - Virtual Environments in the ANUSF VizLab

The VizLab staff, led by Drew Whitehouse, have continued the development of software for the low-cost Virtual Environment system originally created in-house for the WEDGE system built jointly with RSPhysSE in 1998. The software, called pSpace, has been used in producing permanent exhibits for the Powerhouse Museum in Sydney (opened June 1999), the Olympia 'Zeus' exhibit (during the Sydney 2000 Games) and the CSIRO DISCOVERY centre in Canberra (opened in January 2000). The WEDGE system was also demonstrated to guests at the launch of APAC at Parliament House in October 1999.

The kSpace exhibit at the National Museum of Australia (opened March 2001) based on pSpace software with content and technology developed by VizLab staff has been a major success. Visitors design their own fantasy house or vehicle and experience it in a Australian city of the future in a 3D virtual environment. In the first 9 months there were 156,710 interactive sessions run. The estimated total number of visitors was around 230,000 – a staggering figure for an interactive exhibit and a tribute to the careful design by the VizLab team.

In May 1999, the Deputy Vice Chancellor launched the "Borobudur Project" based on a virtual environment model of the eighth/ninth century Buddhist stupa of Borobudur, Java constructed by Dr Ajay Limaye with Professor Mike Greenhalgh, Art History. This is now available on CD, over the internet and in 3-D virtual environment systems at the ANU.

In December 2001, the ANUSF VizLab hosted a highly successful meeting of around 60 researchers, developers and visualization support personnel from around Australia. It was resolved that this would be labelled the first in a series of 'OzViz' meetings and that next year the meeting would be held at the Sydney Vizlab.

Mass Data Storage and the Australian Cooperative Supercomputer Facility (ACSF)

The ANU component of a $1M grant from the Australian Research Council's RIEF Program for 1999/2000 made to the ACSF consortium for mass data storage infrastructure was used for a major upgrade of the University's mass data storage system. This included new tape technology, robotics and a new server and disk cache. These upgrades were extremely useful in providing the capability required to service the data intensive needs of the APAC National Facility.

ACSF was initiated in 1991 by the ANU in conjunction with regional computational consortia representing almost all the New South Wales and South Australian universities. The University of Queensland joined the ACSF in 1997. It was supported by the ARC to provide computational visualization and mass data storage facilities, but has now been superseded by APAC. The ANU agreed to donate its ACSF PowerChallenge to UNSW (to be shared with James Cook University) at the end of 2001.

An additional ANUSF staff member was appointed in 2001 to further extend the user base of the mass data storage system and to work on projects involving data repositories over broadband networks – the 'data grid'.

External Use Scheme

Because of the formation of the APAC National Facility, the External Use Scheme was terminated in 2001. Under this scheme, the ANU made 10 to 15 percent of its supercomputer systems available to other universities free of charge over 13 years. The Scheme typically supported between 110 to 150 researchers at 15 to 20 other universities working on around 50 projects. Details of usage are presented elsewhere in this report.

Computational Science and Engineering Education Program

The Supercomputer Facility and the Department of Computer Science, FEIT, began a special program in education in computational science and engineering in 1996. This program formally ended at the end of 1998, but courses continued in recent years, supported by ANUSF staff (Drs Kahn, Rendell and Singleton). This program has been subsumed in the APAC-supported Education Program.

Fujitsu Research and Development Relationship

The research and development relationship between the Australian National University and Fujitsu Limited entered its fifteenth year in 2001. Under this agreement, the Supercomputer Facility has been involved in a number of software development and research projects, often in conjunction with other sections of the University (including the School of Mathematical Sciences, Computer Sciences Laboratory, RSISE, the Department of Computer Science and the Centre for Resource and Environmental Studies) and in recent years most heavily with the John Curtin School of Medical Research.

As well as participating in the research and technical aspects of these projects, the Supercomputer Facility took overall responsibility for the management of two of the three major areas of the research relationship with Fujitsu. These are the Chemistry and Molecular Modelling project (including a research project in molecular modelling in conjunction with the Computational Molecular Biology and Drug Design Group, John Curtin School of Medical Research) and the Parallel Mathematical Subroutine Library project which terminated in 1999.

Other Activities

Under an agreement with Sun Microsystems from 1999-2001, computational chemistry software was optimised for Solaris systems. This project was transferred to the Department of Computer Science in early 2001.

Dr Gingold was elected Chairman of the Fujitsu International Supercomputer Users Group in 1999 and continues in this position.

Publications

A total of 49 papers by Supercomputer Facility staff members were published in 1999 – 2001. Details are listed elsewhere in this report.

Staff

Head, Academic Services

Robert Gingold, BSc *Monash,* PhD *ANU*

Academic Consultants and Specialist Programmers

Roger Brown, BSc *Melbourne*
Murray Dow, BSc *Monash*, PhD *Tasmania* (half time)
Ben Evans, BSc (Hons) *ANU*, PhD *ANU* **(leader of Systems Administration team)**
Margaret Kahn, BSc (Hons) *Qld,* MSc *Qld,* PhD *ANU* (70% time)
Rika Kobayashi, BSc (Hons) *Sydney*, PhD *Cambridge* (from Jul 2001)
Stuart Midgley, BSc (Hons) *ANU* (from Jun 2001)
Alistair Rendell, BSc *Durham,* PhD *Sydney* (left Jan 2001)
David Singleton, BSc *Monash,* PhD *Monash*

Computational Science & Engineering Program (joint with DCS, FEIT)

Henry Gardner, BSc (Hons) *Melbourne*, Dipl. Comp. Studies *Melb*, PhD *ANU* (left 1999)

Visualization / Virtual Environment Programmers

Stephen Duke, BA *ANU*, MA *ANU* (Jul 2000 - Feb 2001)
Darran Edmundson, BSc (Hons) *University of Waterloo*, PhD *Simon Fraser University* (from Jul 2001)
Ajay Limaye, MSc *Pune*, PhD *Pune*
Stuart Ramsden, GDip *Swinburne*
Drew Whitehouse, BSc *Qld*

Consultant Programmers

Robyn Allsman, BA *UC Berkeley* (half time)
David Houlder, BSc *ANU* (from Oct 2001)
Judy Jenkinson, BSc (Hons) *ANU*, DipEd *CCAE*
Jon Smillie, BSc (Hons) *Qld* (from Oct 2001)

Systems Administrators

Robert Davy, BSc *ANU*
Jonathan McCabe, BSc *ANU*

Administrator

Lee Beatty (left Jan 2000)

Administrator / Scientific Programmer

Cyndy Kelchner, BSc *Grinnell College*, PhD *Iowa State University* (from Sep 2000)

Fujitsu Computational Chemistry Project

Ryan Bettens, PhD (Apr - May 2000)
Andrey Bliznyuk, BSc *Novosibirsk* , PhD *Novosibirsk*
Stephen Greatbanks, BSc *UMIST*, PhD *Manchester* (in JCSMR, left 2000)
Harold Schranz, BSc (Hons) *Sydney*, PhD *Sydney* (left Sep 2000)
Stephen Titmuss, BSc *Wollongong*, MSc *Wollongong* (in JCSMR, left Sep 2001)
Dylan Jayatilaka, BSc (Hons) *WA*, PhD *Cambridge* (Sep 2000 - May 2001)
Vladimir Vassiliev, MSc *Novosibirsk*, PhD *Academy of Sciences of Russia* (from Oct 2001)
Ivan Rostov, MSc *Kazan State University*, PhD *Karpov Institute of Physical Chemistry* (from Jul2001)
Danne Rasmussen, PhD *ANU* (May - Oct 2000)
Thomas Huber, PhD *Swiss Federal Institute of Technology* (left Dec 2000)

Fujitsu Mathematics Project

Lutz Grosz, DipMath *Hanover,* DrRerNat *Karlsruhe* (in SMS, left May 1999)
David Harrar II, BSc *Washington & Lee,* MAM *Virginia,* PhD *Virginia* (in SMS, left May 1999)
Bing Bing Zhou, PhD *ANU* (in SMS/RSISE, left Apr 1999)
Geoff Keating, BSc (Hons) *ANU*, PhD *ANU* (in RSISE, left 1999)

Visiting Fellows

Roger Amos (Aug - Oct 2001)
Harold Schranz (from Sep 2000)
Darran Edmundson (May 1999 - Jun 2001)

Objectives

The Australian National University Supercomputer Facility (ANUSF) was established at the time of the University's purchase of a Fujitsu VP-50/100 vector processor in 1987. The fundamental goals of the Facility are to provide support to researchers and teachers in the application of high performance computing systems through the provision of infrastructure and expertise, including collaborative participation in research and in the promotion to students of the computational approach to problem solving. The high performance computing infrastructure includes visualization and massive data management systems as well as traditional computational platforms.

The ANUSF supports research and teaching staff and postgraduate students at ANU. Facilities are also made available for undergraduate courses. Since 1988 the ANUSF has also supported researchers at other Australian universities under the External Use Scheme and more recently with the APAC National Facility.

The formal objectives of the Facility approved by the Information Technology Strategy Committee are as follows:

> *To provide world-class infrastructure for researchers who require access to HPC systems and ensure that the university remains at the leading edge in its HPC infrastructure and the productive use of HPC systems in support of internationally competitive research programs.*
>
> *To foster the use of HPC systems in new disciplines as well as in areas traditionally dependent on numerically-intensive computation.*
>
> *To promote and implement mechanisms to increase career opportunities for computational scientists, including ANUSF staff, and promote computational science as an applications-*

driven area of academic and computing expertise with a substantial cross-disciplinary nature.

To develop appropriate collaborations with other Australian universities in HPC aimed at sharing the expense and benefits of HPC systems consistent with the University's national role.

To develop, in conjunction with relevant groups, departments and schools, HPC education courses for undergraduates, postgraduates, industry and the community.

To provide a range of other support services and training programs to the High Performance Computing community, e.g. visualization, massive data storage & high-speed networks.

Structure & Management

While the Supercomputer Facility was created with the principal objective of supporting work centred on the supercomputers, its mission now encompasses support and participation in all aspects of advanced computational science in general, including visualization, massive data storage, parallel computing and computational science and engineering education. As a result, the structure of the Facility has changed over the years to reflect this.

The Facility's staff include Academic Consultants, support, systems and visualization programmers and administrators, plus a number of scientific and programming staff engaged on externally funded projects.

The primary responsibility of the Academic Consultants of ANUSF is in the applications area and in establishing an appropriate environment for research requiring high performance computing infrastructure. Contacts with researchers on campus may take a variety of forms, from short consultancies addressing particular questions from users, to extended collaborations in which an Academic Consultant may spend several months as part of a research team implementing an application on the supercomputer. There is also a Programmer who provides general support to the Facility as well as taking on many of the roles of the Academic Consultants.

A lecturer was appointed jointly with the Department of Computer Science, FEIT to develop and deliver Computational Science and Engineering courses to undergraduate and postgraduate students as well as to develop short courses for industry. While this post has now moved full-time to DCS, members of ANUSF staff continue to contribute to the program which is now a component of the APAC-supported Education Program.

The Facility employs Visualization Programmers whose role is to support researchers in the increasingly important area of interpreting the output of large-scale computations and data from other sources such as remote sensors and experiments.

There are two staff who develop software for managing and interacting with large datasets and who also provide applications level support to users of the massive data storage system.

A systems administrator group is responsible for the operational management of the facilities including the supercomputers, the mass storage system, visualization systems, training laboratories and general group workstations.

The Supercomputer Facility has been involved since 1988 in major collaborative projects with computer companies, notably Fujitsu Ltd and to a lesser extent Sun Microsystems. These projects have employed staff in ANUSF as well as JCSMR, the School of Mathematical Sciences and the Computer Science Laboratory, RSISE. These projects are described in more detail elsewhere in this report.

Management Arrangements - High Performance Computing Advisory Committee

The Supercomputer Facility is now a unit of Information Infrastructure Services in the Division of Information. Until 2001 it was advised formally by the High Performance Computing Advisory Committee (HPCAC), which advised the Vice-Chancellor, via the Information Technology Strategy Committee, on all aspects of high performance computing in the research and advanced teaching work of the University and on the development and promotion of computational science disciplines. Following the formation of the Division of Information, a new structure has not yet been established and the HPCAC now acts informally within the terms of reference to:

1. Develop, review and advise on the strategic goals, principles, policies and plans for the development, acquisition, implementation and ongoing support of high performance computing services on campus, particularly those which are centrally provided;

2. Evaluate proposals and plans, and advise on the prioritisation of the needs of staff, students and management involved in research, particularly with respect to the development and implementation of University-wide initiatives and the provision of high performance computing;

3. Make recommendations to the IT Strategy Committee on the resources required for the effective operation of high performance computing;

4. Monitor the service provision for high performance computing;

5. Provide policy and management guidance to the Supercomputer Time Allocation Committee;

6. Provide an annual report to the Vice-Chancellor on progress and achievements in the area of high performance computing in the University;

7. Facilitate initiatives in the computational sciences, particularly those which are interdisciplinary or involve staff working in groups such as the ANUSF;

8. Oversee and promote links and joint activities in computational sciences with industry and other Australian universities;

9. Consider the positioning of the University's high performance computing so that the University may attract a high degree of interest nationally and internationally as a leading research institution.

With the advice of the HPCAC, the Head of ANUSF is responsible for setting goals and developing policy in HPC for the University as well as management of the Facility, its services and internal and external collaborative programs. In its formal role, the HPCAC met 5 times in 1999, 3 times in 2000 and once in 2001.

In 1999-2001 the membership of the HPCAC was as follows:

Chair, appointed by the Vice-Chancellor
Professor J Mould, Director, MSSSO

Chair of Supercomputer Time Allocation Committee
Professor D Evans, RSC (appointed by the Vice-Chancellor)

Members nominated by Chair of IT Strategy Committee, Professor Robin Stanton, PVC (Academic)
Dr G Bicknell, RSAA and SMS
Dr S-H Chung, Chemistry, The Faculties

Members nominated by the Board of the Institute of Advanced Studies
Dr H Gardner, FEIT (and ANUSF, RSPhysSE)
Dr J Gready, JCSMR

Members nominated by the Board of The Faculties
Professor D Williamson, FEIT
Dr T O'Neill, SMS

Student representative (PARSA)
Mr E Mittag, RSC

Representative of IT Services
Dr R Erskine, Director, Information Technology Services

Executive Officer to the Committee
Dr R Gingold, Head, ANU Supercomputer Facility (Ex Officio)

Secretariat
Ms Y Heslop, IT Services and Dr C Kelchner, ANUSF

Supercomputer Time Allocation Committee

Most of the resources offered by ANUSF are subject to allocation by the Supercomputer Time Allocation Committee. Details of the Committee and its activities are presented elsewhere in this report.

Collaboration & Outreach

APAC National Facility

The ANUSF has been charged by the University with the responsibility of servicing the National Facility of the Australian Partnership for Advanced Computing (APAC). This role formally commenced in July 2000 though much planning work began before that date. Under the agreement with APAC, ANU provides accommodation for the national peak supercomputer, access to the mass data storage system and to a lesser extent to the ANUSF VizLab. ANU is also committed to providing over 13 equivalent-full-time staff over three years to support researchers using the system.

ANUSF staff were heavily involved in the acquisition process of the peak system with Dr Gingold (and Professor Evans, RSC) serving on the APAC Technical Evaluation Committee. An initial system installed in August 2000 failed its acceptance tests and APAC determined to reopen the tendering process. This resulted in Compaq being chosen as the supplier and ANU staff, including Professor Stanton, Dr Erskine and Dr Gingold, were involved in the contract negotiations which led to the installation and acceptance of the initial Compaq AlphaServer SC system in April 2001. This underwent a major upgrade in September 2001, ranking the system number 31 in the TOP500 list of supercomputers in the world (Nov 2001), exceeded in power largely by systems in major national laboratories overseas.

The details of the system are described elsewhere in this report. The ANUSF has established extensive documentation on the APAC National Facility web pages (http://nf.apac.edu.au/) including on-line procedures for applying for resources through both the national Merit Allocation Scheme and the Partner shares. ANUSF staff have been active in running courses around the country on using the Compaq system and assisting users with day to day and longer term issues in establishing and optimizing their codes on the system.

By the end of 2001, there were 143 projects on the Compaq SC involving 417 researchers, 374 of whom had usernames on the system. In addition there were 84 ‘start-up’ projects bringing the total number of users to 485.

The total number of researchers associated with projects on the system was 531. ('Start-up' projects are readily available to help researchers familiarise themselves with the system and frame proposals for substantial projects.) Details of non-ANU usage will be published in APAC Annual Reports at http://nf.apac.edu.au.

ANUSF staff also service APAC's Merit Allocation Committee which makes awards of resources on the Compaq SC to researchers around the nation. This involves collating proposals and providing extensive information on system usage and performance to the Committee.

The National Facility, through ANUSF, is also responsible for leading the APAC Centre of Expertise in Computing Tools and Technologies. Dr Kahn is leading this Centre. Dr Russell Standish, UNSW visited in March 2001 to discuss his involvement in this program. Details of its objectives and achievements will be published by APAC.

External Education and Training Activities

In 2001 external education and training activities were conducted as part of our National Facility support role. Introductory courses on using the National Facility were given by ANUSF staff at all APAC Partner sites, with local arrangements facilitated by local support staff. Late in the year an MPI Programming course was developed and delivered in WA and at the ANU. It is planned to be delivered at other sites early in 2002. In total nearly 200 research staff and students attended the courses in 2001, including 140 from outside the ANU. Details are given in the Education and User Training section of this report.

Towards the end of 2001, planning was well underway for an HPC workshop that ANUSF will be running as part of the Summer School in Computational Mathematics. This will involve over 50 graduate students from around the country.

External Use Scheme for Australian Universities (1988-2001)

The External Use Scheme under which the University made available between ten and fifteen percent of the time on its supercomputers was ended in 2001 as a result of the establishment of the APAC National Facility. This Scheme had been very successful and was a factor in the ANU being chosen as the site to host the National Facility. It is therefore worthwhile providing a brief history of the Scheme and its usage in 1999-2001.

Following the acquisition of the first university-based supercomputer in Australia in 1987, the University undertook to provide over ten percent of the capacity of the vector supercomputers free of charge to researchers at other Australian universities. Over the ensuing decade, the External Use Scheme proved very successful. In 1997 it was extended to provide access to the Silicon Graphics PowerChallenge system.

Until 1993, the ANU did not involve itself in deciding the relative merits of projects from external universities. Over the first five years of this External Use Scheme, a formula provided by the Australian Vice-Chancellors' Committee was used to allocate time in bulk to each participating university. By the end of 1992, it was clear that the system needed

modification. The number of projects grew too large, with the result that each project received an inadequate grant. Therefore, after discussions with a number of external coordinators the scheme was altered so that the Supercomputer Time Allocation Committee accepted proposals from external researchers for a reserved percentage of the computer time available. In considering proposals, the Committee was guided by the same principles of academic merit and suitability of the resources to the proposed project as it uses for internal proposals.

In the period since the 1998 ANUSF annual report, there have been 146 researchers (119 with accounts) at 19 universities working on 51 projects. Details of external usage of the ANU facilities are included in the Time Allocation Committee section of this report.

Australian Cooperative Supercomputer Facility (ACSF)

Although now superseded by APAC, the ACSF was a collaborative venture initiated by the ANU in 1991 in conjunction with regional computational consortia representing almost all of the New South Wales and South Australian universities. The University of Queensland joined in 1997.

The ACSF operated with the support of several substantial Australian Research Council infrastructure grants. It was successful in obtaining additional RIEF funding for 1999 from the ARC for a mass data storage initiative. This was used at the ANU to upgrade the mass data storage system (MDSS) with new technology tape drives, improved robotics and a new server and disk array (see elsewhere in this report for details). These upgrades were extremely useful in providing the capability required to service the data intensive needs of the APAC National Facility.

The ACSF originally acquired three identical Silicon Graphics PowerChallenge systems which were installed at UNSW, the University of Adelaide and the ANU. While these systems were never used in a coordinated 'distributed computing' manner, the commonality of systems did lead to a strengthening of ties between support staff and gave access for researchers to software installed in other locations. As with the donation of the older CM5 systems by the ANU and the UNSW to the University of Adelaide, the ANU agreed to deliver its PowerChallenge to UNSW (to be shared with James Cook University) at the end of 2001.

Area 3 – Computational Chemistry Project with Fujitsu Limited

The Area 3 collaborative software development project with Fujitsu Japan was established in 1989 with the aim of porting and optimizing computational chemistry software for the VP-100. The scope of the project was expanded in 1995 to include other mathematical and climate modelling software (in conjunction with DCS and CRES) as well as the preparation of several scientific videos. In 1996 the project was refocussed to concentrate on the porting, optimisation and development of computational chemistry (CC) software for Fujitsu computers, and a joint application research project with Dr Jill Gready (Computational Proteomics and Therapy Design Group, JCSMR) was initiated.

Work undertaken in the project targets both the vector parallel (VPP) and scalar parallel (AP and PrimePower) range of Fujitsu supercomputers. The core software packages of interest to the project in 2001 were GAUSSIAN98 and ADF (Amsterdam Density Functional) quantum chemistry codes, the MOPAC2000 semi-empirical code which includes the MOZYME linear-scaling module, and the AMBER molecular dynamics/ mechanics codes. These packages which are highly tuned by Area 3 team members for Fujitsu supercomputers form the basis for the applications research projects. The project also involves status reports on directions in CC software and applications. Development and applications work on MOZYME generated three additional contracts through the Fujitsu European Centre for Information Technology (FECIT) for implementation of COSMO solvation and a demonstration research project to promote MOZYME's capabilities.

The project has significant contact with Fujitsu personnel. Mr Hiro Hotta, the Fujitsu contact officer for the project, visited ANUSF in April 2000 for discussions based around presentations by the ANUSF staff and JCSMR researchers on the applications projects. The Leader of the Area 3 project also visits Tokyo twice each year to report on the project. An ANU delegation led by Prof Robin Stanton (PVC, Academic) with Dr Bob Gingold (Head, ANUSF), Dr Alistair Rendell (Leader, Area 3) and Dr Jill Gready visited Tokyo in June 2000 for mutual presentations on future directions. For the April 2001 meeting the ANU delegation was expanded to enable discussions on a wider range of topics of interest to Fujitsu: this included Dr Dylan Jayatilaka (Leader, Area 3), Dr Andrey Bliznyuk (ANUSF, MOPAC), Dr Jill Gready (JCSMR, computational biology applications projects), and Dr Roger Amos (ANUSF Visiting Fellow). Dr Gready also visited Fujitsu Laboratories in May 2001 for a presentation and discussion on bioinformatics.

As well as direct contact with Fujitsu Japan a close collaboration exists between the Area 3 work being performed at the ANU and complementary work undertaken by the group led by Dr Ross Nobes, a former ANUSF staff member and now Research Manager at FECIT in the UK. Dr Nobes has also been a collaborator on the MOPAC research project. Dr Nobes visited Fujitsu Japan in October 2001 with Dr Roger Amos (ANUSF Visiting Fellow and Acting Leader, Area 3).

In 2001, Dr Amos took over leadership of the Area 3 project from Dr Jayatilaka, who returned to UWA as an ARC Senior Research Fellow. Dr Rendell and Dr Thomas Huber left the project at the end of 2000 to take up academic positions at ANU and UQ respectively. The project supports four to five other staff working in ANUSF. (Prior to 2001, one post was a postdoctoral fellow, Dr Steve Greatbanks, located in JCSMR.) In 2001, Drs Vlad Vassiliev, Ivan Rostov and Rika Kobayashi joined Dr Bliznyuk in the project team. Dr Cyndy Kelchner also made significant contributions to the project in 2001. Staff are encouraged to collaborate on appropriate research projects with ANU workers. In addition to his direct Area 3 activities, Dr Huber continued his collaboration with Dr Andrew Torda in RSC.

The Area 3 project has also supported the Australian Molecular Modelling Workshops by providing funds for Prof Walter Theil (Marburg, Germany) to speak on semi-empirical QM at MM2000 and for Dr Ursula Rothlisberger (ETH, Switzerland) to speak on Car-Parrinello MD at MM2001.

Since initiated in 1996, the aim of the applications research projects has been to push the CC codes, specifically GAUSSIAN and MOZYME, to the limits of their performance by using them in real large-scale biomolecular research. The work has been undertaken in collaboration with Dr Gready's group in JCSMR. This has proven a very effective way to uncover bugs and inefficiencies in the programs, as well as gaps in desired functionality. The GAUSSIAN-related project (part of STAC project w05) has investigated aspects of substrate and cofactor binding and reaction of the enzyme dihydrofolate reductase (DHFR). The catalytic and ligand-binding mechanisms are of scientific interest because DHFR is a major drug target, but DHFR is also well recognized as a test system because these mechanisms have long proven refractory to experimental and computational investigation. Initial work studying the polarising effect of the enzyme active site on the substrate and cofactor required performing large Hartree-Fock (HF), density functional (DFT) and second-order perturbation theory calculations on systems containing up to 124 atoms and close to 2000 basis functions, within a point-charge field on the remainder of the protein (~3,000 atoms). Further work on the reaction required HF and DFT geometry optimizations for "floppy" active-site fragment complexes representing reactant, transition state and product complexes with up to 71 atoms. However, as such optimizations are poorly and erratically convergent, current work is investigating the usefulness of the ONIOM QM/MM implementation in GAUSSIAN to provide an enzyme-like environment to restrict the search space. Dr Steve Greatbanks worked on this project until mid-2000, and Dr Ivan Rostov from mid-2001. The work has produced three papers and numerous presentations at conferences.

The MOZYME-related research project (STAC project x11) from 1998-2001 was funded by an ARC SPIRT grant to Drs Gready, Rendell and Nobes, with Fujitsu Japan as the industry sponsor. This supported a PhD student, Mr Stephen Titmuss, on an Australian Postgraduate Award Industry (APAI) studentship in JCSMR. His work aimed to investigate the use of MOZYME (a linear-scaling version of MOPAC that has been developed by Dr J.J.P. Stewart with the direct support of Fujitsu) for the study of enzyme reaction mechanisms, and specifically to contrast the use of MOZYME with existing hybrid quantum chemical/molecular mechanical (QM/MM) methods. The results of this work highlighted a number of problems associated with the usability of the MOZYME code, providing valuable feedback to Fujitsu. One such aspect generated two additional contracts from FECIT to implement the implicit solvation model COSMO. The work also revealed several interesting features relating to the interaction of the QM region with the MM region in hybrid calculations and protocols for performing QM/MM calculations. Two papers have resulted directly from this work along with related presentations made by Mr Titmuss, Dr Gready and Dr Rendell at two molecular modeling conferences in Australia and several international conferences, while another paper has resulted from followup of one of the theoretical outcomes. ANUSF's experience with MOZYME led to a collaboration by Drs Bliznyuk and Rendell with another ANU researcher, Dr Shin-Ho Chung, RSPhysSE, on calculation of molecular electrostatic potentials (MEPs) for a protein ion channel, from which two papers resulted. ANUSF's experience also generated a new Fujitsu contract in 2001 (via FECIT) for a demonstration research project using MOZYME which investigated MEPs for prion protein (part of STAC project x04).

Area 3 – Presentations

Dr Bliznyuk gave talks at the MOPAC developers meetings in San Francisco in 2000 and Tokyo in 2001, and presented the following talks at other meetings:

'Mopac2000', Molecular Modelling Workshop MM2001, Canberra, 2001.

'QM/MM and Mozyme calculations of approximate enzyme reaction path', First Mopac User Group Meeting, San Francisco, USA 2000 (with Titmuss SJ, Cummins PL, Rendell AP and Gready JE).

'Linear-scaling Semiempirical Study of Electrostatic Potential Inside Potassium Channel', Molecular Modelling Workshop MM2000, Melbourne, 2000 (with Rendell AP, Allen TW, and Chung SH).

'Accuracy of electrostatic potential in molecular mechanics. Comparison between quantum chemical and molecular mechanical calculations of a protein', Molecular Modelling Workshop, Brisbane, 1999 (with Rendell AP, Allen TW, and Chung SH).

Dr Huber gave the following talks:

'Protein structure prediction: On the cusp between futility and necessity?', The University Queensland Faculty of Engineering, Physical Science and Architecture, Brisbane, September 15, 2000.

'Computer match making in the protein sequence/structure universe', James Cook University, Department of Biochemistry and Molecular Biology, Townsville, May 5, 2000.

'Computational chemistry code performance on the Fujitsu VPP5000', Fujitsu International Supercomputer Users Meeting, National Centre for High Performance Computing, Taipei, October 22, 1999.

'Parallel molecular dynamics on the Fujitsu VPP300', Symposium on High Performance Computing, The Institute of Physical and Chemical Research, Tokyo, March 17, 1999.

'Protein structure prediction: The uncouth and the refined', Competence Centre for Computational Chemistry, ETH, Zurich, January 7, 1999.

Mr Titmuss gave the following conference presentations:

S.J. Titmuss, P.L. Cummins, A.P. Rendell, A.A. Bliznyuk and J.E. Gready. 'Comparison of hybrid quantum mechanical/molecular mechanical and linear-scaling semiempirical QM energy decomposition terms in the interactions of enzyme-ligand complexes.' 7th Australian Molecular Modelling Workshop MM2001, Canberra, October 2001.

S.J. Titmuss, A.A. Bliznyuk, P.L. Cummins, A.P. Rendell and J.E. Gready. 'Comparison of linear-scaling semiempirical and combined quantum mechanical/molecular

mechanical methods applied to enzyme reactions.' 6th Australian Molecular Modelling Workshop MM2000, Melbourne, December 2000.

S.J. Titmuss, J.E. Gready, A.P.L. Rendell and A.A. Bliznyuk. 'Application of linear scaling semiempirical methods to the study of enzyme reaction mechanisms.' 217th American Chemical Society National Meeting (Computers in Chemistry Division), New Orleans, August 1999.

Area 4 – Parallel Mathematical Subroutine Library Project with Fujitsu Limited

This project involved research and development of mathematical library algorithms and code for Fujitsu's VPP parallel-vector supercomputers. The Area 4 project ended at the beginning of the period covered by this report after running for 7 years and producing a state-of-the-art parallel mathematical subroutine library including most commonly used routines across a wide range of applications. The work led to a number of patents being granted.

The Supercomputer Facility managed this project with Dr Margaret Kahn taking responsibility for day-to-day management of the project and the coordination of planning and activities across campus. Academic direction and leadership of the project was provided by Professor Richard Brent, CSL, RSISE and Professor Mike Osborne, Program in Advanced Computation, CMA, SMS. Professor Brent took up a position as Professor of Computing Science at Oxford University but remained involved in the Area 4 project.

Staff and students working on the project were located in SMS, Computer Science Laboratory, RSISE and ANUSF. Three research fellow positions were funded under this project as well as an APA(I) postgraduate student. Geoff Keating, who was supported by an APA(I) postgraduate scholarship supported by Fujitsu, was awarded his PhD in 2000 for his thesis entitled 'Fast Fourier Transforms and the Fujitsu VPP300'.

Area 4 – Publications

M. Hegland, M. Kahn and M. Osborne, A parallel algorithm for the reduction to tridiagonal form for eigendecomposition, Siam Journal on Scientific Computing, 21, pp. 987-1005, 1999.

Lutz Grosz, CTAC99, pp C653-C670, On residual smoothing in ILUM-type preconditioning, 1999.

Chemistry Software Project with Sun Microsystems

A project was begun in mid-1999 with Sun Microsystems (USA) to port and optimize the Gaussian chemistry package for Sun systems. As well as financial support, Sun provided an E3500 system (8 Gbytes memory with eight 400 MHz processors) for the work which was carried out by Dr Rendell. This project is continuing in the Department of Computer Science following Dr Rendell's transfer to a post in that department.

VizLab

Details of the substantial outreach activities by the VizLab are presented in the VizLab section of this report. These may be briefly summarized as follows:

- The holding of the first OzViz workshop in December 2001 attended by 57 researchers and visualization support personnel from around the country, of whom 33 were from outside the ANU.

- The opening in March 2001 of 'kSpace' as a major permanent exhibit at the National Museum of Australia – a highly successful virtual reality experience for children. Dr Darran Edmundson and Drew Whitehouse gave talks at the National Museum in June and July 2001 on the development of the 'kSpace' exhibit.

- The provision of all content and software for a VR exhibit at the CSIRO Discovery centre in Canberra, opened on 1 May 2000.

- The Wedge VR system was displayed at the 1999 Science Festival from 5-9 May.

- The provision of a detailed report on Virtual Environments technology for the Japan Atomic Energy Research Institute to assist the design of systems to help researchers involved in the Earth Simulator project interpret the data coming from the massive 40 Tflops supercomputer expected to be functioning in early 2002. The Earth Simulator project is a major national program by three Japanese government science agencies to make a 'virtual earth' to be used in understanding the earth and predictions of global change (see http://www.es.jamstec.go.jp/).

Special Services to Other Internal and External Organizations

Dr Bob Gingold is currently Chairman of the Fujitsu International Supercomputer Users Group. He served on the Duffield Scholarship Committee at MSSSO. He was Associate Director of the Computational Techniques and Applications Conference CTAC99 held at the ANU in 1999 and served on the advisory committee for the International Symposium on Parallel Architectures, Algorithms and Networks (I-SPAN-99) in Fremantle and on the program committee for HPCAsia 2001 in Queensland.

Dr Gingold was a member of APAC's interim Facilities and Centres of Expertise Committee and he and Dr Robin Erskine served on APAC's Technical Review Group which advised the APAC Board on the acquisition of computers for the National Facility.

Drs Bliznyuk, Jayatilaka, Limaye, Rendell and Rostov served on the organizing committee of the 7th Australian Molecular Modelling Conference, MM2001, held in Canberra.

ANUSF staff prepared and staffed an exhibit for the APAC National Facility at the HPCAsia 2001 conference in Queensland. Contributors included Drs Edmundson, Gingold and Kelchner and Mr Midgley, Ramsden and Whitehouse.

Visitors

Dr Roger Amos of the Chemistry Department, University of Cambridge visited in April 2001 and was a Visiting Fellow at ANUSF from 2 August 2001. Dr Stephen Pickles of Computing Services for Academic Research, CSAR, Manchester Computing, visited in May 2001.

During 2001, there were a large number of visits from staff associated with APAC Partners, including visitors from all states (except SA) and CSIRO.

Other Outreach Activities

On 30 May 2000, a school group from West Wyalong High School (Years 11 and 12) visited the Supercomputer Facility.

Other Activities

The ANUSF has been a sponsor of the annual Australian Molecular Modelling Conferences MM2000 (in Melbourne) and MM2001 (in Canberra) through support of invited speakers.

Roger Brown together with Professor Adrian Gibbs and Dr Mark Gibbs lodged a patent in 2000 entitled “Combinatorial probes and the uses thereof”.

Education & User Training

Seminars and User Training and Information Dissemination

An'Introduction to the APAC National Facility' course was run multiple times around the country in 2001, presented by 8 ANUSF staff with APAC Partners making the local arrangements. The course is intensively 'hands-on' and typically 2 or 3 staff from ANUSF were present at each course. Course dates and locations were as follows:

Date (2001)	Location	Numbers attending
22, 23, 24, 31 May	ANU	> 29
12 July	UNSW / AC3	> 11
24 July	U QLD / QPSF	26
26 July	RMIT / VPAC	14
27 July	RMIT / VPAC	9
27 July	UWA / IVEC	14
20 August	U TAS / TPAC	14
23 August	Vislab / AC3	7
24 August	Vislab / AC3	11
6 September	Bentley Park WA / IVEC	10
30 November	U Newcastle / AC3	12
	TOTAL	**> 157**

Dr David Singleton also delivered an OpenMP and MPI course to 32 attendees from 26-30 June 2000 at the ANU.

A course on MPI Parallel Programming was developed late in 2001 and delivered as follows:

Date (2001)	Location	Numbers
17 September	ANU	8
18 September	ANU	8
19 September	ANU	7
7 December	Bentley Park WA / IVEC	13
	TOTAL	**36**

Each year an introduction to the ANUSF services (in person or via handouts) is presented to new graduate students. In 2001, this was done in February by Drs Kahn and Kelchner.

VizLab staff presented a course on the Houdini visualization software to 8 ACAT staff and students from 5-9 July 1999.

The Supercomputer Facility is also a joint sponsor with CMA, SMS and CSL, RSISE of the weekly *Advanced Computation* seminar series.

Student Supervision

Dr Rendell was on the PhD supervisory panel for Mr Stephen Titmuss from 1998 – 2001. Mr Titmuss' thesis is planned for submission in 2002.

Computational Science and Engineering Education Program (and HPC Laboratory)

The Supercomputer Facility and the Department of Computer Science, FEIT, began a special program in education in computational science and engineering in 1996. This program formally ended at the end of 1998 but courses continued in 1999, supported by ANUSF staff (Drs Kahn, Rendell and Singleton). Drs Kahn and Singleton presented the unit Comp3067 to 30 undergraduate students in second semester 1999. This program has been subsumed in the APAC-supported Education Program. The Supercomputer Facility was toured by a group of undergraduates in this program on 21 May 2001.

In second semester 2001, Drs Alistair Rendell, DCS and Lindsay Hood, Compaq on-site support engineer (at ANUSF), presented a course (COMP4300) on 'Parallel Systems' to six fourth year students using the Facility systems.

Stuart Midgley ran a course for third and honours years students in the Department of Physics and Theoretical Physics, The Faculties, in September 2001 on the FORTRAN language.

Documentation

A substantial effort was made in 2000-2001 to develop a web site for the APAC National Facility. The site http://nf.apac.edu.au/ contains descriptions of the facilities and services

offered, instructions on applying for accounts on the system (including forms for the APAC Merit Allocation Scheme and for each Partner share of the system) and a general guide to HPC resources world-wide. The web site also contains a detailed local user guide to the Compaq AlphaServer SC system written by ANUSF staff.

The ANUSF web site (http://anusf.anu.edu.au/) continues in use largely as a reference point for ANU users.

Users of the facilities are kept informed through 'Notices and News' pages on both the ANUSF and APAC National Facility web pages, with occasional emails to all users. Thus ANUSF no longer produces a printed newsletter.

Publications

The following papers by Supercomputer Facility staff members and closely related staff were published in 1999-2001. Papers by non-ANUSF members of the Fujitsu Mathematics Project and the Computational Chemistry projects are not listed here.

2001

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Staff, Conferences & Training

Staff Changes

ANU Supercomputer Facility Staff

There have been a large number of changes since the last Annual Report.

Dr Cyndy Kelchner joined ANUSF as Administrator/Scientific Programmer from RSBS. Dr Rika Kobayashi (Cambridge University) and Stuart Midgley (UWA) took up Academic Consultant posts and David Houlder, formerly of CRES, was engaged to focus on systems programming tasks associated with the Compaq SC system. Jon Smillie (RSAA) was appointed to work with Robyn Allsman on data intensive and data grid issues.

Dr Darran Edmundson joined the VizLab group, initially as a Visiting Fellow working on the kSpace project for the National Museum. Stuart Ramsden now works half-time for Professor Stephen Hyde's group in RSPhysSE while still located full-time in the VizLab.

There have been a number of staff changes within the Fujitsu Computational Chemistry project during the period of this report. Dr Thomas Huber and Dr Harold Schranz left the project team for posts at the University of Queensland. Dr Danne Rasmussen left for a post in private industry. Dr Alistair Rendell, who led the project for several years until mid-2000, took up a position in DCS in early 2001. Dr Dylan Jayatilaka, a QEII Fellow from UWA, joined the team as leader in 2000 but left to take up an ARC Senior Fellowship in 2001. In 2001 Dr Vlad Vassiliev (Biotechnology Research Institute, Canada) and Dr Ivan Rostov (University of Pennsylvania) joined the team which is now led by Dr Roger Amos (Cambridge University) who will be formally taking up a position at the ANU in early 2002.

Associated Staff

Dr Stephen Greatbanks continued as a postdoctoral fellow in the Computational Molecular Modelling and Drug Design group, led by Dr Gready, JCSMR, to work on the Fujitsu Computational Chemistry project.

Mr Stephen Titmuss, an APA(I) PhD student who was supported by the Fujitsu Area 3 project from 1998 – 2001, plans to submit his thesis in 2002.

Mr Geoff Keating, RSISE, an APA(I) PhD student supported by the Fujitsu Parallel Mathematics Library Software Development project, was awarded a PhD for his thesis 'Fast Fourier Transforms and the Fujitsu VPP300' in 2000. Staff in SMS and RSISE associated with the project (Drs Bing Zhou, David Harrar and Lutz Grosz) left the University in late 1999 after the end of the project in March 1999.

Dr Lindsay Hood, Compaq Consultant, was located on-site at ANUSF from May 2001 under the terms of the contract with Compaq for the National Facility. His presence has been extremely valuable in the successful operation of the National Facility.

Training and Development, Conferences Attended and Talks Presented

Given the unusual and quasi-academic skills required of many of the Facility's staff, suitable development and training is often available only through attendance at conferences and workshops, sometimes necessarily overseas.

2001

Although having formally left ANUSF in January 2001, ANUSF supported Dr Rendell 's visit to Sun Microsystems, Pacific Northwest National Laboratory, USA and Gaussian Inc in February to discuss research collaborations.

Dr Evans, Dr Singleton, Ms Jenkinson and Mr McCabe attended a Compaq training course on 12-13 February 2001 in Melbourne in preparation for the installation of the APAC National Facility system.

Dr Kelchner attended the National Partnership for Advanced Computational Infrastructure 'All Hands Meeting 2001' in San Diego, USA on 25-27 February.

Ms Allsman attended the 18th IEEE Symposium on Mass Storage Systems and Technologies during April in San Diego, USA and presented a paper 'Simplifying the Web User's Interface to Massive Data Sets', Conference Proceedings pp 175-190.

Dr Singleton and Ms Jenkinson attended the Compaq SC user group meeting, CAST, in Paris in May and presented a report on the APAC / ANU site.

Mr Whitehouse visited the National German Research Center for Information Technology, Germany in June to see the work of the Visualization and Media Systems Design group, a pioneering group in projection screen based VR Systems, and also visited the Chalmers University MediaLab, Gothenburg, Sweden where he presented a workshop.

Dr Limaye, Mr Ramsden and Mr Whitehouse attended the SIGGRAPH 2001 conference (28th Annual Conference on Computer Graphics and Interactive Techniques) in Los Angeles, USA in August.

Drs Gingold, Edmundson and Mr Midgley attended the HPC Asia 2001 meeting (5th International Conference and Exhibition on High Performance Computing in the Asia-Pacific Region) in Queensland 24-28 September and staffed two booths in the exhibition – one describing the APAC National Facility and another describing work at ANU in High Performance Computing. Dr Edmundson prepared a demonstration illustrating APAC research work on the National Facility using 3-D video recorded on standard digital video camcorders. Posters and handouts were prepared by Mr Whitehouse, Mr Ramsden and Dr Kelchner.

Drs Bliznyuk, Rostov and Limaye served on the organizing committee of the MM2001 conference (7th Australian Molecular Modelling Workshop) held at the ANU in October. Each of them gave a talk at the conference, as did Dr Jayatilaka.

Ms Allsman attended the AARNet Advanced Internet Workshop in Sydney on 10 October and with Mr Smillie attended the Asia Pacific Grid Forum (ApGRID) 2001 workshop in Tokyo in October.

Dr Bliznyuk gave talks at the Mopac developers meetings in Tokyo in 2001 and presented a paper entitled 'Mopac2000' at the Molecular Modelling (MM2001) conference in Canberra in October.

Dr Gingold attended the linkage to the SC2001 conference (international conference for high performance computing and communications) on 14 November which used the newly installed Access Grid node at the Sydney Vislab.

The VizLab staff and a number of other ANUSF staff attended the first OzViz workshop held at the ANU on 12 December.

In December Dr Edmundson visited virtual reality centres in Korea (KJIST, Kwangju and KAIST, Daejon) and Japan (Media Centre, Osaka and Tokyo Institute of Technology). He gave talks on ANUSF's experiences in 'Creating successful public virtual reality exhibits' and forged new links with Asian VR researchers.

In addition, staff of the VizLab gave a number of other talks and seminars. These are listed in the Visualization and Virtual Environments section of this report.

1999-2000

Several staff attended the ANZIAM one-day seminar on Computational and Applied Mathematics in December 2000 and Dr Singleton attended the SC2000 meeting in Texas, USA in November 2000.

Drs Bliznyuk, Jayatilaka and Rendell attended the Molecular Modelling MM2000 conference in Melbourne in December 2000. Dr Jayatilaka presented a poster on 'Fortran language based object-oriented programming techniques in computational chemistry'. Dr Bliznyuk's talk is listed below.

Dr Gingold attended the FISUM9 meeting in Munich in October 2000.

Mr Davy attended a Sun systems administrator course in Sydney, July 2000.

Drs Gingold and Huber attended the Fujitsu International User Group's annual meeting, FISUM8, in Taiwan in October 1999. Dr Huber presented a talk on 'Computational chemistry code performance on the Fujitsu VPP5000'.

Dr Huber visited the Institute of Physical and Chemical Research, Tokyo, where he presented a seminar on 'Parallel molecular dynamics on the Fujitsu VPP300', at the Symposium on High Performance Computing in March 1999. He also presented the following talks in 1999-2000:

'Protein structure prediction: On the cusp between futility and necessity?', The University Queensland Faculty of Engineering, Physical Science and Architecture, Brisbane, 15 September 2000.

'Computer match making in the protein sequence/structure universe', James Cook University, Department of Biochemistry and Molecular Biology, Townsville, 5 May 2000.

'Protein structure prediction: The uncouth and the refined', Competence Centre for Computational Chemistry, ETH, Zurich, 7 January 1999.

Dr Bliznyuk gave talks at the Mopac developers meetings in San Francisco in 2000 and presented the following talks at other meetings:

'Accuracy of electrostatic potential in molecular mechanics. Comparison between quantum chemical and molecular mechanical calculations of a protein', Molecular Modelling Conference, Brisbane, 1999 (with Rendell, Allen and Chung).

'Linear-scaling Semiempirical Study of Electrostatic Potential Inside Potassium Channel', Molecular Modelling Conference, Melbourne, 2000 (with Rendell, Allen and Chung).

'QM/MM and Mozyme calculations of approximate enzyme reaction path', First Mopac User Group Meeting, San Francisco, USA 2000 (with Titmuss, Cummins, Rendell and Gready).

During 1999-2000 Dr Rendell made a number of visits to Japan associated with the Fujitsu Computational Chemistry project:

October 2000	Harp meeting, Nagoya University, RIKEN (Dr Jayatilaka also attended this meeting.)
March 2000	HARP meeting (Fujitsu) and RIKEN
January 2000	Nagoya University and Institute for Molecular Science (IMS)
October 1999	Harp Meeting (Fujitsu)
Jun/Jul 1999	Makuhari Labs (Fujitsu)
March 1999	Harp meeting (Fujitsu)

Dr Rendell also visited Sun Microsystems in April 1999 and visited the San Diego Supercomputing Center where he gave a talk entitled 'Computational Chemistry on Fujitsu Parallel Supercomputers'.

A number of ANUSF staff were involved in organizing and presenting at the CTAC'99 conference held at the ANU in September 1999. Dr Singleton presented on 'Using C++ for Scientific Computation' at an HPC Workshop associated with the conference. At an associated Scientific Visualization Workshop, Mr Whitehouse and Mr Ramsden presented papers on 'Virtual Environments' and 'Crystallography and Hyperbolic Geometry – A Visualization Case Study'.

Mr Ramsden and Mr Whitehouse attended the Association for Computing Machinery Special Interest Group in Graphics (SIGGRAPH 99) in Los Angeles, USA in August 1999.

Seminars and Lectures by Non-ANUSF Staff

A seminar on the OpenMP programming model was conducted for ANUSF and around 20 other ANU staff by Mr George Delic of HiPERiSM Consulting in October 1999. ANUSF organized Dr Marie Christien Sawley of ETH, Switzerland to give a seminar in DCS on 'The HPCC Supercluster' in November 1999.

Professor Jack Donagarra gave an ANU Public Lecture in September 1999 on 'High Performance Computing and Trends'.

Other Travel

Dr Gingold accompanied Professor Stanton and Dr Jill Gready, JCSMR, on a visit to Fujitsu Ltd, Japan in June 2000 to discuss joint research programs and emerging technologies.

Visualization Laboratory

VizLab – Visualization and Virtual Environments Laboratory

Scientific visualization is the generic name given to techniques that use images and animations to interpret scientific data. Although not restricted to supercomputing applications, initially the field was largely driven by the difficulty of interpreting the enormous amounts of data produced by many supercomputer applications. Such data are often not only massive but multi-dimensional and time dependent and so conventional graphics techniques are often completely inadequate. The Facility's initiative in scientific visualization began in 1990 with the appointment of a Visualization Programmer. The main aim of the VizLab is to provide software support and visualization expertise and advice to users of advanced computers rather than as a generally accessible 'graphics work area'. Nevertheless, researchers and postgraduate students are able to use the VizLab's high-end visualization workstations and other equipment. In many cases researchers have used the VizLab's facilities to help decide upon the optimum solution to their visualization requirements before purchasing personal and departmental systems.

The Visualization Laboratory currently houses the following major equipment:

- Silicon Graphics Onyx Reality Engine (RE2) workstation
- Intergraph ZX-10 with dpsReality video hardware
- Stereo-enabled CRT projectors and 3D magnetic tracking system for group Virtual Environment applications

The VizLab programmers have moved from desktop SGI O2s to PCs in a general shift away from high cost hardware systems. A combination of commercial, public domain and home grown software is used. The main software systems are Houdini (Side Effects) for high quality modelling and animation, AVS (Advanced Visual Systems) for general scientific visualization and dpsVelocity for video compilation and recording. In

addition the pSpace software developed by VizLab staff is used to drive the stereo-virtual environments system and larger WEDGE systems.

Virtual Reality Installations

The 1998 ANUSF Annual Report introduced the Wedge Project with RSPhysSE, where the VizLab was responsible for the designing and programming of a low-cost PC-based multi-wall immersive environment which in its 2-walled configuration has been named 'The Wedge'. As a result of the publicity generated by this project, the VizLab has subsequently been contracted to develop four interactive and/or immersive PC-based systems for installation in public spaces. These projects have been conducted on a commercial basis, in particular the National Museum of Australia project which involved several staff in a major project over an extended period of time.

Powerhouse Museum Wedge (January 1999)

Following a successful demonstration at Sydney's Powerhouse Museum in November 1998, the Powerhouse commissioned the VizLab to develop a program of scientific visualization content to run on a Wedge screen configuration, a component of the award winning 'Universal Machine' exhibition (recently renamed 'Cyberworlds: computers and connections'). The program features a number of scientific visualizations produced by ANU researchers. The system allows viewers to move in the space around and inside the geometric models using a joystick.

CISRO Discovery Centre (January 2000)

A seven minute, non-interactive Wedge presentation was developed showcasing CSIRO research into biochemistry, plant industry, mining and radio astronomy. The Discovery Centre was officially opened by Prime Minister John Howard who personally viewed the stereographic content. Dr Darran Edmundson joined the VizLab for this project and has since taken on a continuing position with ANUSF.

Powerhouse Museum Olympia 'Zeus' Exhibit (August 2000)

The VizLab produced an interactive stereographic presentation of a 3D model of a Zeus statue (provided by University of Melbourne) on a dual screen configuration as part of the Powerhouse Museum's Olympic exhibit at the time of the Sydney Olympic Games.

National Museum of Australia 'kSpace' Exhibit (March 2001)

The VizLab was commissioned to build a major new high-tech interactive exhibit for the Children's Gallery of the new National Museum of Australia. The project was designed and implemented by VizLab and casual staff over a fourteen month period. The exhibit encourages children to 'imagine the future' by having them design their own futuristic buildings and vehicles followed by a computer graphic ride through an Australian-themed 'city of the future' which is populated with their own inventions. This is projected on a large single-screened 3D VR system using the pSpace technology developed for the Wedge system.

The exhibit has been very successful. In the first 9 months there were 156,710 interactive sessions run. The estimated total number of visitors was around 230,000. The exhibit has featured on many Australian television programs covering the new National Museum.

Software Developed

A Win32 stereo movie player was developed for the display at the HPC Asia 2001 conference.

The 'pSpace' software, developed to drive multi-screen virtual environment displays using PC or SGI graphics systems, continues to be developed and upgraded to Optimizer release 1.31. As well, a VRML viewer has been built upon pSpace. A large amount of custom code was developed for the kSpace exhibit at the National Museum of Australia with software copyright retained by the ANU.

The 'pScene' software was developed to export animations from Houdini into the pSpace environment, initially used for the CSIRO Discovery Centre VR theatre.

Service Provided

Visualization and consultation support was provided to researchers in a wide range of ANU schools including CRES, RSES, RSC, RSPhysSE, Psychology, Art History, JCSMR, Department of Chemistry, Department of Applied Mathematics (RSPhysSE), Department of Theoretical Physics (RSPhysSE) and ACAT.

The following is a description of some of the larger projects undertaken recently:

- Cover image for *Nature* to go with article by Mick Collins, RSC. Published 3 November 2000, Vol. 290 Number 5493 (April 2000)
- Ying Qiao - 3 images for PhD thesis and paper submitted to *Nature* (June 2000)
- Dr Shin-Ho Chung, Chemistry, Calcium Channel Animation (July 2000)
- Simon Tursk - 4 stereo images for the CSIRO magazine *The Helix* Number 75 December 2000/January 2001 (October 2000)
- Images for a paper by Dr Malcom Sambridge, RSES, 'Finding acceptable models in nonlinear inverse problems using a neighbourhood algorithm', Inverse Problems, 17 (2001) 387-403, Institute of Physics Publishing (February 2001)
- Volume visualization of paper sample scanned at BASF, Germany for Dr Mark Knackstedt, Department of Applied Mathematics (September 2001)
- Setup of pSpace environment for Summer Scholar doing work on relaxation of crystallographic structures at Department of Applied Mathematics, RSPhysSE (December 2001)

- Centre for Resource and Environmental Studies terrain modelling and management plan visualization of the Ben Chifley catchment area (with Mr Chris Buller and Professor Tony Jakeman). This work is continuing.
- School of Psychology, 'motion-in-depth' studies conducted in VizLab's pSpace virtual environment with Dr Mark Edwards. This work is continuing.
- Work is in progress on a package with the Geoseismic research group, RSES, to look at earth tomography and try to reconstruct the interior of earth from seismic data.

A 14 minute video 'Permeation and Selectivity of the Calcium Channel' was produced for Dr Shin-Ho Chung (RSPhysSE). Voltage gated calcium channels perform a number of important biological functions, such as stimulating the contraction of skeletal and cardiac muscle. To do this they must be able to select out just calcium ions from amongst the much more abundant sodium, potassium and chloride ions, whilst still passing millions of ions each second. The video illustrates the work of Shin-Ho Chung and his group in this area. They employ electrostatic calculations and Brownian dynamics simulations to find the properties of the channel.

A 24 minute video production 'Permeations of Ions across the Potassium Channel' was produced for Shin-Ho Chung (RSPhysSE). The movie presents the results of the theoretical calculations by Dr Chung and his group. Using the recently unveiled structure of the Potassium Channel they employ a combination of electrostatics, Brownian dynamics and molecular dynamics to study how the channel discriminates between potassium and sodium ions, and reproduce some physiological attributes of conduction.

First OzViz Workshop

A Visualization and Virtual Reality Workshop was organized by the VizLab staff in December 2001, with assistance from Dr Kelchner . This two-day workshop for Australian researchers and support staff in the fields of virtual reality and visualization was attended by 57 people from around Australia (33 from outside the ANU). The workshop involved a large number of talks and demonstrations of VE systems at ANUSF and DCS. As a result of the success of the workshop, attendees agreed to make it an annual event for the community entitled 'OzViz'. The OzViz 2002 meeting will be held at the Sydney Vislab. VizLab staff created a web site for publishing proceedings of the meetings (http://anusf.anu.edu.au/Vizlab/ozviz/).

Seminars, Talks and Courses Presented

VizLab staff presented a 4-day course on the Houdini visualization software to 8 staff and students in ACAT in July 1999.

Conferences attended given by VizLab staff are listed elsewhere in this report. Talks given by VizLab staff include the following:

‘Creating Successful Public Virtual Reality Exhibits,’ Kwangju Institute of Science and Technology, Kwangju, Korea. (Edmundson, December 2001)

‘Creating Successful Public Virtual Reality Exhibits,” Invited Talk, Nabi, Seoul, Korea. (Edmundson, December 2001) - a government gallery and research centre focused on the application of digital media to art and culture in the 21st century.

‘Diverse Visualization Techniques Across the Mesoscale Domain’, Visualization and VR Workshop, ANU. (Ramsden, December 2001)

‘Taking VR to the Public’, Visualization and Virtual Reality Workshop, ANU. (Edmundson, December 2001)

‘kSpace: How it was built’ (delivered to primary school children), National Museum of Australia. (Whitehouse, May 2001)

‘kSpace: Production of an interactive virtual reality exhibit’, National Museum of Australia. (Whitehouse, June 2001)

‘kSpace: From Concept to Fruition’, National Museum of Australia. (Edmundson, July 2001 and August 2001)

‘kSpace’, Chalmers University MediaLab, Gothenburg Sweden (Whitehouse, June 2001)

‘AVS’, 2-day workshop, Chalmers University MediaLab, Gothenburg Sweden (Whitehouse, June 2001)

‘kSpace’, GMD - National German Research Center for Information Technology (Whitehouse, June 2001)

‘Visualization and the pSpace/Wedge Virtual Environment at the ANU’, The Bureau of Meteorology Research Centre Workshop. (Whitehouse, November 1999)

Other Activities

Stuart Ramsden was involved in a successful Linkage Infrastructure proposal with $480,000 awarded to the project ‘Bioscope IV: Advanced Scanned Probe Microscopy’ including a haptics/AFM component. Chief Investigators: Senden, Craig, Parker and Ramsden (September 2001).

Dr Edmundson produced a six minute stereo-video promotional movie for display at the APAC booth at the HPC Asia 2001 conference in Queensland, September 2001.

An interactive 3D presentation of scientific visualization models was presented at the official opening of APAC at Parliament House in October 1999 using a portable Wedge.

Dr Limaye produced a detailed report on Virtual Environments technology for the Japan Atomic Energy Research Institute to assist the design of VE systems for the major Japanese national Earth Simulator project.

A demonstration of graphics and VR systems was given to 65 Youth Science Forum Students from Australia and overseas schools on 18 January 2001.

Drew Whitehouse gave a presentation on the kSpace installation to the ACT Division of the Australian Academy of Technological Sciences and Engineering in December 2001.

Mass Data Storage System

History and System Development

The Mass Data Storage System (MDSS) was acquired in 1993 to support data intensive projects. The MDSS has since been upgraded with faster transfer rate, lower latency and higher capacity improvements. The original system used an early Hierarchical Storage Management product that was later replaced by the current software SAM-FS from LSCI/Sun. This software has improved over time, with a number of LSCI/ANU collaborations spawning modifications to the software. These upgrades have kept the Mass Data Storage System up to world class standards. Additional details of the current configuration of the fileserver, tape systems and network connections are found elsewhere in this report.

Access to the MDSS is mainly through locally modified utilities which enable the transfer and interrogation of data from jobs running on the supercomputers in a safe way. These utilities are undergoing further development to continue to improve the integration of the peak systems.

Standard transfer tools such as 'ftp' and 'scp' are used, plus some minimal use of NFS across campus. An additional tool, Bulkstage, optimises throughput during the bulk retrieval of files from MDSS.

Management Policy, Usage and Consultancy

The storage system is managed and accounted using a project based system. The majority of MDSS users are also using the APAC National Facility, and to assist in the management and accounting of these projects the same project codes from the APAC National Facility Compaq SC are used on the MDSS. APAC users with specific data intensive needs are able to get direct access to the mass data storage system along with a small home area. Other APAC users are only able to access the system through utilities installed on the Compaq SC. Other ANU mass data projects use the system independent of the APAC National Facility and have a small home area as well as a shared project space.

The local configuration has been tailored to provide archive tape redundancy to avoid lost files caused by a damaged tape, robustness in the face of system problems, optimisation according to file characteristics, and transparent operation with respect to naive users.

The MDSS is not intended to replace group or departmental disks due to the different I/O characteristics required. Details of the access policy are published on the ANUSF website. The Mass Data Store is also available to users of the APAC system and therefore has a MAS and Partner usage scheme.

During the first year of operation of the APAC National Facility, usage of the MDSS gradually grew to 90 active projects accessing approximately 17 TBytes of data in total. Over 2 TBytes of this usage was from non-ANU users of the APAC National Facility. Requests for space have increased dramatically as APAC projects have started to realise the potential of the integration of high performance computation and large data storage facilities.

Projects dealing with massive amounts of data need to carefully consider all aspects of data acquisition, storage, retrieval, navigation, and interpretation before using the MDSS. In addition to the ANUSF consultants and programmers, an MDSS programmer helps to develop special utilities for projects with specific requirements. In recent times this development has included web analysis utilities for MSSO data archives and web interfaces to be used in the various Astronomy Virtual Observatory projects.

Major Installed Hardware & Software

Major Installed Hardware and Software

APAC National Facility Compaq AlphaServer SC

The Compaq AlphaServer SC was installed in two major stages during 2001. Stage 1 consisted of 46 ES40 systems each with 4 GBytes of memory and 72 GBytes of disk (a total of 184 Alpha EV67 667 Mhz processors) connected by a Quadrics switch, and over 2 TBytes of shared disk. The production service commenced on 30 April 2001. A 16 processor GS system was added in July. The system was reduced in size in October during the transition to the final hardware configuration which consists of 120 ES45 nodes, each with four 1 GHz Alpha EV68 processors and at least 4 GBytes of memory, for a total of 480 processors. The production service on the upgraded system commenced on 30 October 2001.

An aggregate disk capacity of 7.2 TBytes is devoted to job specific scratch space (/jobfs) which is distributed amongst the nodes. Most nodes have 60 GBytes and a smaller number of nodes have larger scratch space, up to a maximum job scratch space of 200 GBytes on a node. Access to the CPUs, memory, and job scratch space is controlled via the PBS queueing system through a resource request, and the data and resources are released automatically at the end of the job.

The nodes of the system are connected via a Quadrics switch, forming an integral part of the Compaq SC configuration. Each node of the system, up to a maximum capacity of 128 nodes, are connected to the Quadrics switch. The switch architecture is based on a fat tree, which provides low latency and high bandwidth connections nearly uniformly between any two nodes. While IP emulation is available, the switch uses a proprietary protocol which is used by the Compaq SC MPI library to sustain a high bandwidth, low latency interconnect at an application level. The switch is also used as part of the distributed filesystem, providing access to home directories and short term directories transparently to all nodes.

The operating system used on the SC is based on Compaq's fully 64 bit Tru64 operating system. The fully 64 bit architecture means that there is no

confusion for the user about whether to link to a 32 bit or 64 bit library. Utilities are available to assist in the transition to 64 bit code, and our experience has been that these utilities have, where needed, been adequately addressing home-grown codes.

The modified Tru64 operating system for the SC platform includes the distributed filesystem technology, and a low level resource management system called RMS. For the APAC National Facility a locally modified version of Veridian's PBS queue management system has been developed to integrate with the underlying RMS system. In addition the modified PBS system provides more functionality, allowing for better control of resource requests and assistance with tailoring the system to local configuration needs. Some of the modifications include:

- project accounting
- allocation of CPU resources
- management of job scratch spaces
- job suspension for high priority and parallel jobs
- intelligent job scheduling
- integration with software network license tokens
- control of software usage, consistent with agreements with software suppliers

Many of the management controls can be modified as required by the needs of individual projects or usernames.

The above modifications have involved considerable effort by ANUSF staff and have ensured that the system is very efficiently used and that work is distributed on the system in a manner which favours parallel jobs. A substantial effort has also gone into gathering data and reporting on system utilisation.

Fujitsu VPP300

The VPP300 is an aircooled, vector supercomputer from Fujitsu, with 13 processing elements (PEs) providing a peak speed of almost 30 Gflops. Each vector unit can achieve a peak speed of 2.2 Gflops and is connected via a full crossbar network with a peak bandwidth of 570 MBytes per second bi-directional and an achievable latency of about 5 microseconds. Installed in 1996, the VPP300 was take out of general service in June 2001 but continues to be operated for special projects and to support selected users.

The Fujitsu VPP300 has 14 GBytes of memory with 5 PEs having 2 GBytes, the remaining 8 PEs with 0.5 GBytes. Two of these PEs provide I/O capability.

Silicon Graphics PowerChallenge

The ACSF PowerChallenge system at ANUSF is a CMOS Shared Multiprocessing (SMP) supercomputer with twenty 195 MHz MIPS R10000 superscalar processors. The PowerChallenge has a peak speed of 7.8 Gflops. Installed in 1996, it was taken out of

general service in July 2001 and donated to ACSF partner UNSW at the end of 2001 to share spare parts with James Cook University.

Alpha-Linux Cluster

The Alpha-Linux Cluster (named wyrd) was installed in 1998. It consists of twelve 533 MHz Alpha LX164s each with 256 MB of memory and 5.3 GBs of IDE disk connected by a fast ethernet switch. The Alpha was chosen for its price/performance in floating computations with sustained performance far better than Pentium chips.

It has been heavily used by the Supercomputer Facility to support selected users and as a development platform for some of the software on the APAC National Facility system.

High Performance Computing Laboratory

The High Performance Computing Laboratory (HPCLab) was handed over to DCS in 1999. The HPCLab was a teaching laboratory established by ANUSF in the CSIT building as part of the Facility's joint Computational Science and Engineering education program with the Department of Computer Science.

Mass Data Storage System

The Mass Data Hierarchical Storage System (MDSS) is comprised of several components. The last major upgrade was in 1999 with the installation of new technology tape drives, new robotics and a new file server and disk cache.

The front-end ('store', accessible to users over the network as store.anu.edu.au) is a Sun E6500 with six 400 MHz Ultrasparc II processors and 1 GB of memory, with a large I/O capacity for effectively managing a large number of disks, high speed tape devices and network interfaces. The storage system is coupled to the APAC National Facility Compaq SC by a private network, the traffic being routed over the high speed SC Quadrics network and then forwarded over a gigabit connection to store. The system is also connected to the ANU network over a shared 100 Mbit network connection, and separately to the regional network (RNO) via a 100 Mbit network connection.

The MDSS has 0.5 TByte of Sun A3500 hardware RAID-5 disk array connected to the front-end via four SCSI connections, which is used as cache for the data management system. The system also has 50GB of dedicated disk scratch and variable longer term scratch areas inside the disk cache for larger scratch needs. The disk cache is separated into several filesystems depending on the characteristics of the dataflow for each project on the Compaq SC. These filesystems are NFS mounted by each of the four filesystem server nodes of the Compaq SC system which, in turn, share the filesystems to all of the compute nodes. The filesystems allow each project to access their data simply as /massdata/projectid.

The Mass Data Storage System has a total storage capacity of 300 TBytes on the current media. The tape system consists of a StorageTek Powderhorn Robotic Tape Silo (6000 tape capacity) with the tape drives listed below.

- 8 StorageTek 9840 tape drives
  - 20 MBytes/sec transfer rate
  - 20 GBytes per tape
  - 12 second latency to data
- 2 StorageTek Redwood tape drives
  - 11 MBytes/sec transfer rate
  - 50 GBytes per tape
  - 65 second latency to data

Several tape drives are connected to both the main system and an experimental SAM-FS development system using a StorageTek SN3200 fibre/SCSI bridge and SN2000 fibre hub.

The Hierarchical Storage System is managed using Sun/LSCI's SAM-FS software. This software manages the data storage devices including the allocation of data to disks, the data connectivity over the SCSI connections, the tape allocation, and the transparent movement of data between disk cache and tape silo. Two copies of each project's data are written to separate tape pools in the library, to guard against failure of the magnetic media. All data undergo hardware compression through the drives as they are written to tape. APAC National Facility data are written to the 9840 tape drives for better reliability and the much lower latency time to access data.

Collaborations between ANU Supercomputer Facility staff and LSCI have resulted in several new enhancements of the migration software. These include mechanisms for improving tape management, migration control, and robustness of the system. Future work is directed at allowing several servers to be used as a cluster at the front-end rather than having a single point of failure. Collaboration with StorageTek and LSCI has also resulted in the inclusion of technology for sharing tape drives over a fibre SAN through the ACSLS library management control station.

In 2002 the disk cache is expected to be replaced with a high speed fibre connection and much larger capacity. The tape system will be upgraded with next generation high density tape drives to replace the current Redwood tape drives and media. The connectivity of the system to the ANU, AARNet and GrangeNet networks will also be improved with the implementation of Gigabit networking. The capacity, performance and accessibility of the system will therefore be significantly increased to meet the growing demands on the system.

Software Installed on the Systems

Full details of software on systems operated by ANUSF can be found on the WWW at http://anusf.anu.edu.au/software/ and http://nf.apac.edu.au/facilities/. Packages available during 2001 were as listed below. (Note that access to some packages is restricted, e.g. to users who also have their own individual license for the package.)

Chemistry & Biology

ACES II
ADF
Amber
CHARMM
CNSsolve
Gamess
Gaussian
Molden
Molpro
MOPAC2000
NW-Chem
Q-Chem

CFD & Engineering

ABAQUS
CFX
Fluent
(LS-DYNA on order)

Climate Modelling

CCM3
POM

Mathematics

BLACS
BLAS
CPML
CXML
FFTW
IMSL
LAPACK

Maths (continued)

Maple
Mathematica
Matlab
NAG
PetSC *
R Statistical Package
Scalapack
Parallel Programming Libraries/Tools
MPI
Global Array (GA) Tools
GNU Pthreads
PVM

Compilers

Fortran - F77, F90,
F77/OpenMP, F90/OpenMP
C and C++, C/OpenMP

Debuggers & Profilers

Ladebug
Totalview
Vampir and Vampirtrace
Electric Fence

Code Development Utilities

CVS
xdiff
xxdiff

File Formats & Data Bases

HDF5
netCDF

Network Access

Ssh
Vnc

Editors

GNU Emacs
Vim

Scripting Languages

Perl
Python
Tcl/Tk

Graphics

GMT
GnuPlot
IDL
Mesa
NCAR Graphics
Pgplot
Renderman

Time Allocation Committee & ANU Usage

The Supercomputer Time Allocation Committee (STAC) has had the responsibility for allocating time on the University's production high performance computing systems since 1987.

The Committee's policy is that all but small start-up allocations of time to local researchers should be subject to a peer-review process. Applicants are required to provide an academic justification for the amount of time requested, as well as information by which the suitability of the computer system for the proposed research can be judged. The Chair of the Committee obtains reports on proposals from referees throughout Australia and in many cases from overseas. New projects and continuing projects that make large requests for resources are routinely refereed. The Committee makes grants of time on the basis of these reports and on the effective use of previous grants. Since the time between meetings of the Committee is quite long, procedures are implemented to assist researchers who wish to commence projects that evolve between meetings of the Committee.

Given the mature nature of the bulk of the projects, the process has been relatively informal in recent years.

Membership of the Time Allocation Committee

Members of the Committee are academics appointed on a rotating basis by the Chair. The Chair is appointed by the Vice-Chancellor. Members are as follows:

Professor Denis Evans, Research School of Chemistry (Chair)
Professor Martin Bennett, Research School of Chemistry
Dr Stephan Marcelja, Research School of Physical Sciences and Engineering
Dr Geoff Davies, Research School of Earth Science
Dr Brian Molinari, Department of Computer Science, FEIT
Dr Bob Gingold, ANUSF (ex officio)

Allocations to ANU Projects on the Fujitsu VPP300 and SGI PowerChallenge systems for 1999-2001

Overall there were 87 projects involving 199 researchers of whom 176 had usernames on the Fujitsu VPP300 and SGI PowerChallenge systems.

The allocations and usage are listed below by computer system used. Some projects use more than one system. The tables present a summary of the number of researchers, time allocations and usage for each project, plus tables showing the overall breakdown by subject area. Grants are allocated in Service Units. A Service Unit is related to CPU use and the priority of the job; at normal priorities, one Service Unit corresponds to one hour of CPU time on a single processor.

Internal Fujitsu VPP300 Allocations and Usage

A total of 43 internal VPP300 projects were approved by the Time Allocation Committee. During 1999-2001, there were 157 researchers associated with ANU projects on the VPP300, comprising 43 Principal Investigators and 142 individual user accounts on the system.

Table 1 lists the details for each project. Detailed descriptions of the projects are presented in Appendix A. (The totals obtained by summing the columns headed 'Number of Researchers' in the following tables are greater than 157 because some researchers work on more than one project.)

The system was heavily used throughout 1999-2001 before decommissioning in June 2001. Note that time was also used by external users, for systems development and for the Fujitsu collaborative software development projects and similar activities.

Table 2 presents a breakdown of allocations by subject for 2000, the most recent full year of operation.

Internal SGI PowerChallenge Allocations and Usage

A total of 65 projects involving 43 Principal Investigators and 156 associated researchers were awarded allocation with 139 connected users. Of these projects, 40 were also allocated time on the VPP system. The system was heavily used throughout 1999-2000 though there was some tapering off before decommissioning in July 2001.

Table 3 lists the details for each project. Descriptions of the projects are presented in Appendix A.

Table 4 presents a breakdown of allocations by subject for 2000, the most recent full year of operation.

ANU Allocations on the APAC National Facility Compaq AlphaServer SC in 2001

The ANU has a formal 'Partner Share' of 41% of the APAC National Facility Compaq SC. In addition, researchers have access to the APAC national Merit Allocation Scheme. The total resources allocated and used by ANU researchers were somewhat over 50% of the overall system in 2001.

Table 5 lists projects on the APAC National Facility Compaq SC system that were awarded time in 2001 under the ANU's share of the system. There are 50 projects involving 147 associated researchers with 134 having usernames on the system.

Figure 1 shows the breakdown by research field for projects with allocations under ANU's share of the system.

Table 6 lists those projects led by ANU researchers which received APAC Merit Allocation Scheme awards in 2001. These 7 projects involved 44 researchers with a total MAS allocation of 92,229 SU. Details of these projects can be found in Appendix A (or on the APAC National Facility website).

Figure 2 shows the breakdown by research field for ANU researchers with allocations under the APAC national Merit Allocation Scheme.

Allocations to External Projects for the Fujitsu VPP300 and SGI-PC Allocations for 1999-2001

As outlined in the Collaboration and Outreach section of this annual report, the STAC continued to take responsibility for allocating the bulk of external usage of the VPP300 and the SGI-PowerChallenge during 1999 - early 2001. Projects from 19 universities were supported. There were 42 external projects on the VPP300 and 16 on the SGI PowerChallenge, with a total number of 146 researchers involved in the projects, 119 having usernames on the machines.

Tables 7 and 8 list these projects' allocations and usage. In contrast with previous years, detailed descriptions of individual projects are not given because it was felt that it would unnecessarily burden external researchers to request research reports for both this annual report and APAC reports.

Table 1: ANU Principal Investigators — Grants and Usage on VPP300 in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Ahrling K A	**(Chemistry, Faculty of Science)**			
q63	Theoretical Studies of the Oxygen Evolving Site of Photosystem II	1	385	147
Allen T W	**(Chemistry, Faculty of Science)**			
w50	Molecular Dynamics Studies of Membrane Ion Channels	5	8320	8282
Bachor H A	**(Physics and Theoretical Physics, Faculty of Science)**			
x09	Optical Homodyne Tomography	2	25	0
Baxter J N	**(Systems Engineering, RSISE)**			
v62	Automatic Feature Learning for OCR and Speech Recognition	2	50	0
Bicknell G V	**(Astronomy, RSAA)**			
w57	Simulation of Astrophysical Jets	2	1110	2
x28	Simulation of Twisted Flux Tubes	4	500	55
Blackwell B D	**(Plasma Research Laboratory, RSPhysSE)**			
k05	Computational Support of the H-1 Heliac	5	30	0
Braun J	**(Geodynamics, RSES)**			
m22	Three-dimensional Modelling of Crustal Deformation Coupled to Surface Processes	4	2375	4
Brent R P	**(Computer Sciences Laboratory, RSISE)**			
k58	Applications of Integer Factorization	3	5000	5101
Chelvanayagam G	**(Human Genetics, JCSMR)**			
x06	Mechanism of the GSTT2 Enzyme	3	175	0
x07	Flexibility of the GSTT2 Enzyme	3	825	14
Chung S H	**(Chemistry, Faculty of Science)**			
r06	Permeation of Ions Through Membrane Channels – Molecular Dynamics Studies	7	71628	64398
x26	Simulation of Biological Ion Channels	7	19118	17967
Collins M A	**(Physical and Theoretical Chemistry, RSC)**			
s01	Molecular Potential Energy Surfaces by Interpolation	6	1750	984
Cummins P L	**(Computational Molecular Biology, JCSMR)**			
u51	qm/MM Calculations on Solvated Molecules	4	9500	4334

Table 1 (continued): ANU PIs — Grants and Usage on VPP300 in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Davies G F	**(RSES)**			
k43	Mantle Convection	1	75	0
r01	Mantle Plumes	2	550	158
Dewar R L	**(Theoretical Physics, RSPhysSE)**			
s55	Plasma Turbulence in 3-Dimensional Magnetically Confined Plasmas	7	4100	369
Easteal S	**(Human Genetics, JCSMR)**			
w02	Comparative Evolutionary Analysis of Mitochondrial Genomes Using Maximum Likelihood	3	100	0
Edmundson D E	**(Optical Sciences Centre, RSPhysSE)**			
x12	Dynamics of Partially Coherent Solitons	2	325	71
Ennis-King J P	**(Physical and Theoretical Chemistry, RSC)**			
x05	Electrokinetic Transport Properties of Ionic Systems	2	200	57
Evans D J	**(Physical and Theoretical Chemistry, RSC)**			
s02	Calculation of the Stability of Phase Space Trajectories using Molecular Dynamics Simulations	5	11600	2832
Fischer G	**(Chemistry, Faculty of Science)**			
u01	Energies and Potential Surfaces of the Excited Electronic States of the Triazines	2	2525	1570
u54	Structures and Vibrational Frequencies of Pure Halocarbon Clusters, and Mixed Clusters with Water	2	2725	2270
Gardner H J	**(Theoretical Physics, RSPhysSE)**			
k12	3D MHD Equilibrium and Stability	5	3150	1424
Gorbatov A	**(Seismology, RSES)**			
d76	Tomographic Imaging of the Western Pacific	1	200	1
Gready J E	**(Computational Molecular Biology, JCSMR)**			
u53	Definition of the Chemical Mechanism of the Photosynthetic Enzyme Rubisco	6	16625	12360
v53	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Lactate and Malate Dehydrogenase	3	8800	4587
w05	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Dihydrofolate Reductase	5	10850	2530
x04	Simulation of the Structure of Sugar Chains of Glycoproteins	4	17300	13178

Table 1 (continued): ANU PIs — Grants and Usage on VPP300 in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
x11	Evaluation of the Potential of MOZYME for the Study of Enzyme Reaction Mechanisms	3	5300	2812
Gulacsi M	**(Theoretical Physics, RSPhysSE)**			
x18	The Density Matrix Renormalization Group	3	550	1
Hall P G	**(Mathematics Research Section, SMS)**			
w12	Estimating the Components in a Mixture of Two Smooth Regression Curves	2	50	2
Heath G A	**(Inorganic Chemistry, RSC)**			
x30	Electronic Structure Calculations via ANUSCF	1	600	0
Houwing F P	**(Physics and Theoretical Physics, Faculty of Science)**			
v59	Planar Laser-Induced Fluorescence Imaging of Hypervelocity Flows; Computer Simulation and Sensitivity Analysis	6	150	1
Kennett B L	**(Seismology, RSES)**			
s52	Highly Nonlinear Solitary Waves in Compressible Fluids	3	625	212
x14	Surface Wave Tomography	2	1375	231
Kuyucak S	**(Theoretical Physics, RSPhysSE)**			
x15	Investigation of Continuum Approaches to Modelling of Membrane Channels	4	11228	11260
x16	Investigation of Anharmonic Phonon Excitations in Collective Nuclei	3	100	0
Lindesay J A	**(Geography, SREM)**			
s13	Modelling the Atmospheric Response to Mid-Latitude Forcing During Enso	2	1300	178
Nix H A	**(CRES)**			
q56	Environmental Domain Analysis with Very Large Data Sets —Evaluation of Attributes, Weightings, Classificatory Strategies	2	200	20
Ollis D L	**(Protein Structure, RSC)**			
s06	Protein Refinement and Engineering	9	220	1
Petrie S A	**(Physical and Theoretical Chemistry, RSC)**			
w60	Ab Initio and Molecular Dynamical Studies on Systems of Chemical and Astrochemical Interest	3	100	18

Table 1 (continued): ANU PIs — Grants and Usage on VPP300 in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Radom L	**(Computational Quantum Chemistry, RSC)**			
k29	Gas-Phase Ion Chemistry	14	10920	9758
p03	Unusual Structural and Energetic Consequences of Ionization	4	9730	5076
q07	Chemistry of Free Radicals	3	7185	3061
q08	Theoretical Thermochemistry	2	7130	3352
r54	Planar Carbon	2	7675	5616
s08	Free Radical Polymerization Reactions	2	6220	2790
v01	Enzyme-Mediated Reactions	2	7730	4209
v55	Ion-Neutral Complexes	3	2595	394
v56	Small Ring Phosphorus Chemistry	3	4720	3302
Savage C M	**(Physics and Theoretical Physics, Faculty of Science)**			
r62	Modelling Atomic Diffraction	3	790	203
Schranz H W	**(Physical and Theoretical Chemistry, RSC)**			
s10	Efficient Calculation of Statistical and Dynamical Reaction Rates for Large Dimensional Molecular Systems	1	235	179
Smith H B	**(Plasma Research Laboratory, RSPhysSE)**			
w03	Modelling Low Pressure, Low Temperature Discharges using Particle-in-cell Techniques	4	25	0
Stranger R	**(Chemistry, Faculty of Science)**			
x24	Magnetic Interactions in Transition Metals	2	2500	1
Sutherland R S	**(Astronomy, RSAA)**			
v60	The Impact of Realistic Plasma Cooling Processes on the Hydrodynamics of Astrophysical Shockwaves	2	3400	1194
Taylor J A	**(CRES)**			
m33	A 3-D Tropospheric Transport and Chemistry Model	6	50	0
Weiss A A	**(Statistics, Faculty of Economics)**			
x25	Bayesian Analysis on the Reserve Bank of New Zealands Macroeconomic Model	1	50	33
Welberry T R	**(Physical and Theoretical Chemistry, RSC)**			
p05	Computation of X-ray Diffraction Patterns for 3D Model Systems	4	1125	470
Wickramasinghe DT	**(Mathematics, Faculty of Science)**			
w56	Accretion Disks Around Black Holes in Compact Binaries	4	100	0

Table 1 (continued): ANU PIs — Grants and Usage on VPP300 in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Williams J S	**(Electronic Materials Engineering, RSPhysSE)**			
x03	Molecular Dynamics Simulation of Defects in Ion Implanted and Annealed Silicon	4	1800	681
Totals*			**295694**	**197750**

* Totals include projects not listed here which made little or no use of the grant.

Table 2: Allocations by Research Field — Grants on VPP300 in 2000

Research Field	Researchers	Grant	Percent
Biomolecular Modelling	36	29920	27
Bioscience and Environmental Science	2	100	0
Chemistry	24	29705	27
Molecular Dynamics and Statistical Physics	20	40838	37
Geophysics and Earth Science	12	1825	2
Mathematics, Computer Science and Systems Engineering	4	2000	2
Plasma Research	9	2150	2
Other Physics and Astrophysics	13	2570	2
Sociology and Economics	2	50	0
Total		**109158**	

Table 3: ANU Principal Investigators — Grants and Usage on SGI-PC in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Allen T W	**(Chemistry, Faculty of Science)**			
w50	Molecular Dynamics Studies of Membrane Ion Channels	5	7000	7537
Baxter J N	**(Systems Engineering, RSISE)**			
v62	Automatic Feature Learning for OCR and Speech Recognition	2	50	0
Braun J	**(Geodynamics, RSES)**			
m22	Three-dimensional Modelling of Crustal Deformation Coupled to Surface Processes	4	2125	563
Brent R P	**(Computer Sciences Laboratory, RSISE)**			
k58	Applications of Integer Factorization	3	5000	5401
Chelvanayagam G	**(Human Genetics, JCSMR)**			
x06	Mechanism of the GSTT2 Enzyme	3	1500	921
x07	Flexibility of the GSTT2 Enzyme	3	1200	869
Chung S H	**(Chemistry, Faculty of Science)**			
w16	Analysis of Single Channel Currents Using Signal Processing Techniques Based on Hidden Markov Models	5	25400	22388
x26	Simulation of Biological Ion Channels	7	15000	13455
Collins M A	**(Physical and Theoretical Chemistry, RSC)**			
s01	Molecular Potential Energy Surfaces by Interpolation	6	12260	10037
Cummins P L	**(Computational Molecular Biology, JCSMR)**			
u51	qm/MM Calculations on Solvated Molecules	4	18120	16546
Dewar R L	**(Theoretical Physics, RSPhysSE)**			
s55	Plasma Turbulence in 3-Dimensional Magnetically Confined Plasmas	7	150	0
Easteal S	**(Human Genetics, JCSMR)**			
w02	Comparative Evolutionary Analysis of Mitochondrial Genomes Using Maximum Likelihood	3	4800	51
El-Khoury W	**(Mathematics, Faculty of Science)**			
x23	Black Hole Soft X-Ray Transients	1	1200	0
Ennis-King J P	**(Physical and Theoretical Chemistry, RSC)**			
x05	Electrokinetic Transport Properties of Ionic Systems	2	700	0

Table 3 (continued): ANU PIs — Grants and Usage on SGI-PC in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Evans D J	**(Physical and Theoretical Chemistry, RSC)**			
r61	Strain Rate Dependence of Heat Transfer as Applied to Planar Poiseuille Flow	2	18000	12087
s02	Calculation of the Stability of Phase Space Trajectories using Molecular Dynamics Simulations	5	22700	16168
Fischer G	**(Chemistry, Faculty of Science)**			
u01	Energies and Potential Surfaces of the Excited Electronic States of the Triazines	2	4900	4146
u54	Structures and Vibrational Frequencies of Pure Halocarbon Clusters, and Mixed Clusters with Water	2	4550	4159
Gibson F W	**(Membrane Biochemistry, JCSMR)**			
q11	A Combined Molecular Biological and Computer Graphics Study of Biologically Active Proteins	2	20	5
Gready J E	**(Computational Molecular Biology, JCSMR)**			
u53	Definition of the Chemical Mechanism of the Photosynthetic Enzyme Rubisco	6	15125	13259
v53	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Lactate and Malate Dehydrogenase	3	8400	6910
v54	Computation of Electron Densities of Proteins by a Classical Electrostatic Model	2	11900	11009
w05	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Dihydrofolate Reductase	5	11600	10300
x04	Simulation of the Structure of Sugar Chains of Glycoproteins	4	13950	11010
x11	Evaluation of the Potential of MOZYME for the Study of Enzyme Reaction Mechanisms	3	11400	8949
Gulacsi M	**(Theoretical Physics, RSPhysSE)**			
x18	The Density Matrix Renormalization Group	3	8500	2897
Hall P G	**(Mathematics Research Section, SMS)**			
x21	Curve Estimation	3	5100	2336
Heath G A	**(Inorganic Chemistry, RSC)**			
x30	Electronic Structure Calculations via ANUSCF	1	600	135
Jakeman A J	**(CRES)**			
s31	Dynamic Separation of Catchment Water Balance	3	50	0

Table 3 (continued): ANU PIs — Grants and Usage on SGI-PC in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Kheifets A S	**(Electron Physics Unit, RSPhysSE)**			
x01	Non-perturbative Theory of Atomic Ionization with Two-electron Continuum	1	3100	444
Knackstedt M A	**(Applied Mathematics, RSPhysSE)**			
w09	Large-scale Modeling of Multi-phase Flows in Heterogeneous Porous Media	8	24285	19648
Kreger T	**(ACAT)**			
v57	Batch Rendering of Computer Animated Sequences	2	15073	3662
Lilley T	**(Seismology, RSES)**			
v63	Electrical Conductivity Structure of the Australian Continent	3	25	0
Lindesay J A	**(Geography, SREM)**			
s13	Modelling the Atmospheric Response to Mid-Latitude Forcing During Enso	2	100	0
Marrink S	**(Applied Mathematics, RSPhysSE)**			
w10	Computation of Surface Forces	2	500	0
Martin J P	**(Laser Physics Centre, RSPhysSE)**			
w08	Strongly Driven 2,3,6 Level Quantum Systems	1	2500	894
McClelland D	**(Physics and Theoretical Physics, Faculty of Science)**			
x19	Ligo Gravitational Wave Data Analysis	6	1000	9
Ollis D L	**(Protein Structure, RSC)**			
s06	Protein Refinement and Engineering	9	1505	635
Pace R J	**(Chemistry, Faculty of Science)**			
v64	ab initio Modelling of the Manganese Centre of Photosystem II	2	2850	1435
Petravic J	**(Physical and Theoretical Chemistry, RSC)**			
x31	Transport Properties of Systems With Long Range Interactions	1	7000	4280
Petrie S A	**(Physical and Theoretical Chemistry, RSC)**			
w60	Ab Initio and Molecular Dynamical Studies on Systems of Chemical and Astrochemical Interest	3	300	165

Table 3 (continued): ANU PIs — Grants and Usage on SGI-PC in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Radom L	**(Computational Quantum Chemistry, RSC)**			
k29	Gas-Phase Ion Chemistry	14	14150	11281
p03	Unusual Structural and Energetic Consequences of Ionization	4	12775	8137
q07	Chemistry of Free Radicals	3	12421	7879
q08	Theoretical Thermochemistry	2	10365	3822
r54	Planar Carbon	2	11030	6734
s08	Free Radical Polymerization Reactions	2	10830	6199
v01	Enzyme-Mediated Reactions	2	7096	5973
v55	Ion-Neutral Complexes	3	6245	3652
v56	Small Ring Phosphorus Chemistry	3	5835	5233
Ramsden S J	**(ACAT)**			
x17	Rendering Computer Animated Representations of Scale	1	2000	0
x22	Rendering of Nanotechnology Computer Animation Sequences	1	2700	0
Sambridge M S	**(Seismology, RSES)**			
r58	Applications of Computational Geometry to Large Scale Geophysical Inverse Problems	1	1290	31
Savage C M	**(Physics and Theoretical Physics, Faculty of Science)**			
u57	Quantum Trajectories in Atom Optics	3	300	5
w17	Relativistic Optics	3	200	0
x27	Bose-Einstein Condensates and Atom Lasers	3	1400	513
Schranz H W	**(Physical and Theoretical Chemistry, RSC)**			
s10	Efficient Calculation of Statistical and Dynamical Reaction Rates for Large Dimensional Molecular Systems	1	245	217
Stranger R	**(Chemistry, Faculty of Science)**			
x24	Magnetic Interactions in Transition Metals	2	4500	2191
Taylor J A	**(CRES)**			
m33	A 3-D Tropospheric Transport and Chemistry Model	6	50	0
Torda A E	**(Inorganic Chemistry, RSC)**			
v04	Development and Application of Protein Fold Recognition Force Fields	4	4500	1740
w51	Blending Protein Secondary Structure Information and Knowledge-Based Force Fields	3	5000	2423
x08	NMR Spectral Assignment Using Structural Information	3	2000	108

Table 3 (continued): ANU PIs — Grants and Usage on SGI-PC in 1999 - 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Weiss A A	**(Statistics, Faculty of Economics)**			
x25	Bayesian Analysis on the Reserve Bank of New Zealands Macroeconomic Model	1	4100	2348
Welberry T R	**(Physical and Theoretical Chemistry, RSC)**			
p05	Computation of X-ray Diffraction Patterns for 3D Model Systems	4	760	42
Wickramasinghe DT	**(Mathematics, Faculty of Science)**			
w56	Accretion Disks Around Black Holes in Compact Binaries	4	1200	25
Totals*			**410530**	**280863**

* Totals include projects not listed here which made little or no use of the grant.

Table 4: Allocations by Research Field — Grants on SGI-PC in 2000

Research Field	Researchers	Grant	Percent
Biomolecular Modelling	40	45880	28
Bioscience and Environmental Science	0	0	0
Chemistry	30	48539	30
Molecular Dynamics and Statistical Physics	16	33400	21
Geophysics and Earth Science	14	10925	7
Mathematics, Computer Science and Systems Engineering	10	12400	8
Plasma Research	7	25	0
Other Physics and Astrophysics	16	8420	5
Sociology and Economics	2	3100	2
Total		**162689**	

Table 5: ANU Principal Investigators with Allocations under ANU Partner Share — Grants and Usage on APAC National Facility Compaq SC in 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Becker N	**(Nat Cen for Epidemiology and Pop Health)**			
x00	Estimating Trends in HIV Incidence for Australian Women	2	1000	709
Bicknell G V	**(Astronomy, RSAA)**			
x28	Simulation of Twisted Flux Tubes	4	529	101
Braun J	**(Geodynamics, RSES)**			
m22	Three-dimensional Modelling of Crustal Deformation Coupled to Surface Processes	4	625	1
Chung S H	**(Chemistry, Faculty of Science)**			
r06	Permeation of Ions Through Membrane Channels - Molecular Dynamics Studies	10	102649	104660
x26	Simulation of Biological Ion Channels	9	92189	95315
Collins M A	**(Physical and Theoretical Chemistry, RSC)**			
s01	Molecular Potential Energy Surfaces by Interpolation	9	4293	1663
Cummins P L	**(Computational Molecular Biology, JCSMR)**			
u51	QM/MM Calculations on Solvated Molecules	4	17864	18064
Davies G F	**(Geodynamics, RSES)**			
r01	Mantle Plumes	2	264	0
Evans D J	**(Physical and Theoretical Chemistry, RSC)**			
r61	Strain Rate Dependence of Heat Transfer as Applied to Planar Poiseuille Flow	2	14760	2816
s02	Calculation of the Stability of Phase Space Trajectories Using Molecular Dynamics Simulations	5	26000	22545
Fischer G	**(Chemistry, Faculty of Science)**			
u01	Energies and Potential Surfaces of the Excited Electronic States of the Triazines	2	2476	947
u54	Structures and Vibrational Frequencies of Pure Halocarbon Clusters, and Mixed Clusters with Water	2	2246	1303
Fux R M	**(Astronomy, RSAA)**			
x42	Simulations of Spiral Galaxies	4	1500	0
Gardner H J	**(Theoretical Physics, RSPhysSE)**			
k12	3D MHD Equilibrium and Stability	5	1890	1962

Table 5 (continued): ANU Principal Investigators with Allocations under ANU Partner Share — Grants and Usage on APAC NF Compaq SC in 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Gorbatov A	**(Seismology, RSES)**			
d76	Tomographic Imaging of the Western Pacific	1	904	412
Gready J E	**(Computational Molecular Biology, JCSMR)**			
u53	Definition of the Chemical Mechanism of the Photosynthetic Enzyme Rubisco	6	21192	16739
v53	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Lactate and Malate Dehydrogenase	2	3863	2052
w05	Hybrid Quantum Mechanical and Molecular Mechanical Studies of the Reaction Mechanism of Dihydrofolate Reductase	5	17294	10387
x04	Simulation of the Structure of Sugar Chains of Glycoproteins	4	26020	9600
x11	Evaluation of the Potential of MOZYME for the Study of Enzyme Reaction Mechanisms	3	15208	3589
Gulacsi M	**(Theoretical Physics, RSPhysSE)**			
x18	The Density Matrix Renormalization Group	3	31235	27087
Hall P G	**(Mathematics Research Section, SMS)**			
x21	Curve Estimation	3	1436	438
Isaev A V	**(Centre for Bioinformation Science, JCSMR)**			
x36	A Rigorous and Efficient Method for Inferring Phylogenetic Relationships	2	25000	11063
Kalyanasundaram S	**(Engineering, FEIT)**			
x33	Finite Element Modelling of Engineering Systems	5	1150	0
Kennett B L	**(Seismology, RSES)**			
x14	Surface Wave Tomography	2	157	0
x35	Simulation of Seismic Wave Propagation Using a Wavelet-Based Method	2	7000	6721
Kheifets A S	**(Electron Physics Unit, RSPhysSE)**			
x01	Non-perturbative Theory of Atomic Ionization with Two-electron Continuum	1	959	332
Knackstedt M A	**(Petroleum Engineering, University of NSW)**			
w09	Large-scale Modeling of Multi-phase Flows in Heterogeneous Porous Media	8	24875	24226

Table 5 (continued): ANU Principal Investigators with Allocations under ANU Partner Share — Grants and Usage on APAC NF Compaq SC in 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
McClelland D	**(Physics and Theoretical Physics, Faculty of Science)**			
x19	Ligo Gravitational Wave Data Analysis	8	7292	308
Meriaux C A	**(Geophysical Fluid Dynamics, RSES)**			
x47	Plume Zonation and Modelling with Fluent	1	1010	564
Ollis D L	**(Protein Structure, RSC)**			
s06	Protein Refinement and Engineering	9	284	43
Petravic J	**(Physical and Theoretical Chemistry, RSC)**			
x31	Transport Properties of Systems with Long Range Interactions	1	22600	20648
Radom L	**(Computational Quantum Chemistry, RSC)**			
k29	Gas-Phase Ion Chemistry	16	36370	15313
p03	Unusual Structural and Energetic Consequences of Ionization	4	4600	2450
q07	Chemistry of Free Radicals	3	4139	1408
q08	Theoretical Thermochemistry	2	2760	6
v56	Small Ring Phosphorus Chemistry	3	1609	1326
Rendell A P	**(Computer Science, Faculty of Science)**			
x32	Development of Computational Chemistry Methods for Parallel Processors	2	1400	407
Sambridge M S	**(Seismology, RSES)**			
r58	Applications of Computational Geometry to Large Scale Geophysical Inverse Problems	1	367	1
Savage C M	**(Physics and Theoretical Physics, Faculty of Science)**			
x27	Bose-Einstein Condensates and Atom Lasers	3	276	2
Saxton C J	**(Astronomy, RSAA)**			
x34	Filamentary Structure in the Lobes of Radio Galaxies	3	690	677
Schranz H W	**(Physical and Theoretical Chemistry, RSC)**			
s10	Efficient Calculation of Statistical and Dynamical Reaction Rates for Large Dimensional Molecular Systems	1	300	81
Smola A J	**(Computer Sciences Laboratory, RSISE)**			
x46	Kernel Methods for Bioinformatics	4	10000	2783

Table 5 (continued): ANU Principal Investigators with Allocations under ANU Partner Share — Grants and Usage on APAC NF Compaq SC in 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Stranger R	**(Chemistry, Faculty of Science)**			
x24	Magnetic Interactions in Transition Metals	5	4109	1080
Torda A E	**(Inorganic Chemistry, RSC)**			
v04	Development and Application of Protein Fold Recognition Force Fields	4	2168	1199
w51	Blending Protein Secondary Structure Information and Knowledge-Based Force Fields	3	1304	317
x08	NMR Spectral Assignment Using Structural Information	3	1484	484
Welberry T R	**(Physical and Theoretical Chemistry, RSC)**			
p05	Computation of X-Ray Diffraction Patterns for 3D Model Systems	4	848	347
Wickramasinghe D T	**(Mathematics, Faculty of Science)**			
x40	Structure of Accretion Discs in Close Interacting Binaries	2	500	94
Williams D R	**(Applied Mathematics, RSPhysSE)**			
x20	Collapse and Folding of Block Copolymers	2	1900	1751
Totals*			**550588**	**414021**

* Totals include projects not listed here which made little or no use of the grant.

Figure 1: Allocations under ANU Partner Share on APAC NF Compaq SC — Breakdown by Research Field in 2001

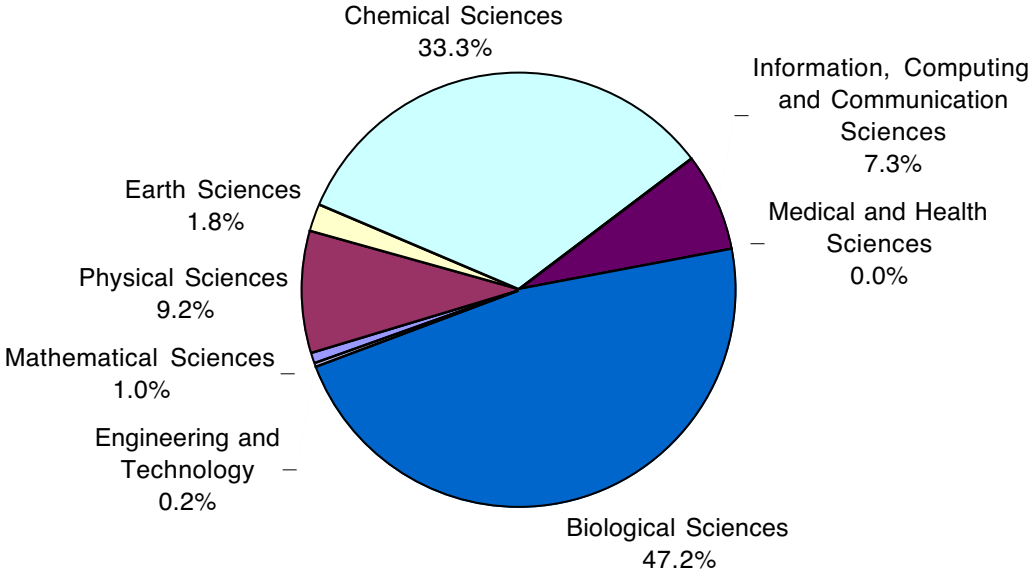

Figure 2: Merit Allocation Scheme Allocations to ANU Principal Investigators on APAC National Facility Compaq SC - Breakdown by Research Field in 2001

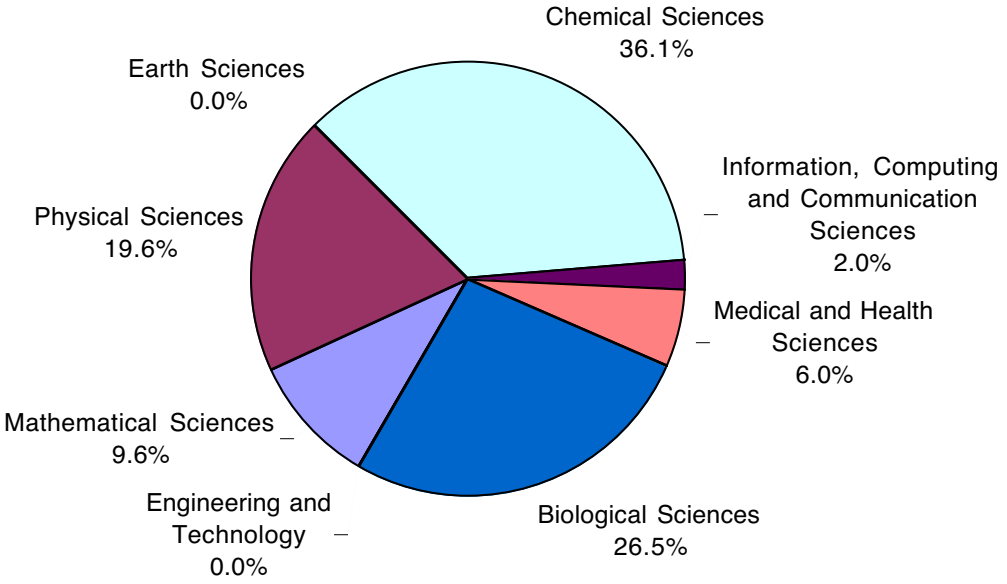

Table 6: ANU Principal Investigators with Merit Allocation Scheme Allocations — Grants and Usage on APAC National Facility Compaq SC in 2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Chung S H	**(Chemistry, Faculty of Science)**			
d32	Simulation of Biological Ion Channels	7	12778	14261
Cummins P L	**(Computational Molecular Biology, JCSMR)**			
d52	QM/MM Studies of Enzyme Reaction Mechanisms	4	12778	12793
Gready J E	**(Computational Molecular Biology, JCSMR)**			
d55	Definition of Chemical Mechanism of the Photosynthetic Enzyme Rubisco and MD Simulation of Glycoproteins	10	20444	12903
Hall P G	**(Mathematics Research Section, SMS)**			
d33	Fault Line and Boundary Estimation from Spatial Data	4	8889	723
Radom L	**(Computational Quantum Chemistry, RSC)**			
d39	Structural and Mechanistic Chemistry	10	13129	12908
Savage C M	**(Physics and Theoretical Physics, Faculty of Science)**			
d66	Atom Lasers and Bose-Einstein Condensates	5	18111	16354
Torda A E	**(Inorganic Chemistry, RSC)**			
d97	Protein Structure Prediction, New Force Fields, New Methods	6	6100	4330
Totals*			**92229**	**74272**

* Totals include projects not listed here which made little or no use of the grant.

Table 7: External Principal Investigators — Grants and Usage on VPP300 in 1999-2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Banner M L	**(Mathematics, University of NSW)**			
h01	Modelling Spectral Dissipation in the Evolution of Wind Waves	2	2200	1493
Bisset D K	**(Mechanical Engineering, University of Newcastle)**			
g91	The AGE Method for DNS of Turbulent Shear Flows	1	1935	998
Blackburn H M	**(Building, Construction and Eng, CSIRO)**			
g89	Spectral Element Methods For Turbulent Flow Simulation	4	11290	8688
Bursill R J	**(Physics, University of NSW)**			
h04	Density Matrix Renormalisation Group Studies of Quantum Lattice Models	5	7240	2734
Coutis P F	**(Centre in Stat Science and Ind Math, Queensland University of Technology)**			
h21	Numerical Modelling of Island Wakes in Deep and Shallow Water	2	1310	702
Cranny T R	**(Charles Sturt University)**			
h06	Density Classification	2	900	391
Daivis P J	**(Applied Physics, Royal Melbourne Institute of Technology)**			
g73	Molecular Rheology of Freely Jointed Chain Model Polymer Melts	3	2550	2267
Denier J P	**(Mathematics, University of Adelaide)**			
h11	Viscous Secondary Instabilities in Boundary Layer Flows	3	1550	43
Djenidi L	**(Mechanical Engineering, University of Newcastle)**			
h30	Wall Turbulence Management by Roughness and Active Control	2	900	323
England M H	**(School of Mathematics, University of NSW)**			
h25	A Global Ocean Model Intercomparison Project	4	1250	337
Esselle K P	**(Electrical and Computer Engineering, Macquarie University)**			
g78	Human Organ Dosimetry Exposure to Radio and Microwave Fields	4	1750	210
h29	Antenna Analysis and Design Using Advanced Numerical Electromagnetic Techniques	3	750	3

Table 7 (continued): External PIs — Grants and Usage on VPP300 in 1999-2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Flambaum V	**(School of Physics, University of NSW)**			
h22	Many-Body Theory and Violation of Fundamental Symmetries	8	510	14
Hamer C J	**(Department of Physics, University of NSW)**			
g57	Study of Spin Lattice and Lattice Gauge Theory	6	6076	2355
Harrowell P	**(Dept of Chemistry, University of Sydney)**			
g79	The Characteristic Length of Slow Dynamics in a Glass-forming Binary Mixture	3	2776	1924
Haymet A D	**(School of Chemistry, University of Sydney)**			
g59	Molecular Dynamics Simulations of Solutes in Liquid Water and at the Ice/Water Interface	3	2200	1400
Hocking G C	**(Maths and Stats, Murdoch University)**			
h24	Two-Layer Withdrawal from Reservoirs	2	900	222
Holloway P E	**(Geography and Oceanography, University of NSW)**			
g69	Modelling Tidal Generation of Internal Waves in The Ocean	3	4011	1317
Hush N	**(Theoretical Chemistry, University of Sydney)**			
h27	Investigations of an Efficient Catalytic Mechanism Involving Platinum Complex Dimers	3	2050	1185
Leslie L M	**(School of Mathematics, University of NSW)**			
h09	A New High Resolution Non-Hydrostatic Atmospheric Model	3	1750	592
Middleton J F	**(Mathematics, University of NSW)**			
h00	Ocean Circulation of the Great Australian Bight	3	2750	1019
Middleton J H	**(Mathematics, University of NSW)**			
h02	Modelling Coastal Ocean Processes	6	5701	4521
Pitman A J	**(Department of Physical Geography, Macquarie University)**			
g96	Base Simulations Within Global Soil Wetness Project	2	4120	4046
Sadus R J	**(School of Information Technology, Swinbourne University of Technology)**			
g36	Molecular Simulation of Phase Transitions	6	6690	2551

Table 7 (continued): External PIs — Grants and Usage on VPP300 in 1999-2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Soria J	**(Mechanical Engineering, Monash University)**			
h26	Coherent Structure Evolution in a Turbulent Channel Flow	2	4500	659
Stelbovics A T	**(Physics, Murdoch University)**			
h15	Direct Approach to Electron-Impact Excitation/Ionisation of Hydrogen	2	2000	418
Storer R G	**(Department of Physics, Flinders University)**			
e80	Resistive Magnetohydrodynamics for Heliac and Stellarator Plasmas	2	760	227
Von Nagy-Felsobuki E I	**(Dept of Chemistry, University of Newcastle)**			
g19	Rovibrational Calculations of Helide Ions	4	3750	1551
Wang X H	**(School of Geography and Oceanography, University of NSW)**			
h12	A Numerical Study of Ocean Circulation in the South China Sea	1	1650	546
Willett G D	**(School of Chemistry, University of NSW)**			
h14	Vanadium Oxide Cluster Anion Calculations – Optimized Structures and Reactivity with Small Organic Molecules	2	1660	1144
Yates B F	**(Department of Chemistry, University of Tasmania)**			
g29	Theoretical Studies on the Mechanism of the Stevens Rearrangement and Related Reactions	3	7070	4442
Totals*			**98241**	**48328**

* Totals include projects not listed here which made little or no use of the grant

Table 8: External Principal Investigators — Grants and Usage on SGI-PC in 1999-2001

Project Code	Project Title	Number of Researchers	SU Awarded	SU Used
Bowie J H	**(Chemistry, University of Adelaide)**			
g77	Structures and Reactivities of Unusual Anions and Neutrals	6	9300	6588
Cheetham N W H	**(Chemistry, University of NSW)**			
h20	Modelling Studies on Carbohydrate Hydration	2	2750	2283
Esselle K P	**(Electrical and Computer Engineering, Macquarie University)**			
g78	Human Organ Dosimetry Exposure to Radio and Microwave Fields	4	1200	112
Liddell M J	**(Chemistry Department, James Cook University)**			
g92	Atmospheric Chemistry - Dimethyl Sulphate Formation	2	1100	48
Lim K F	**(Biological and Chemical Sciences, Deakin University)**			
g72	Simulation Studies of Collisional Deactivation in Combustion-Model and Atmospheric-Model Systems	4	8670	6506
Meyer K	**(Animal Genetics and Breeding Unit, University of New England)**			
h31	Estimating Genetic Covariance Functions For Lifetime Growth of Beef Cattle	1	1800	54
Pitman A J	**(Department of Physical Geography, Macquarie University)**			
g96	Base Simulations Within Global Soil Wetness Project	2	73	24
Robson R E	**(Physics Dept, James Cook University)**			
h10	Electron Transports in Gases	3	40	11
Schulte J	**(Applied Physics, University of Technology, Sydney)**			
g66	Quantum Molecular Dynamics of the Formation of Large Carbons	4	570	60
Uren N F	**(Dept of Exploration Geophysics, Curtin University of Technology)**			
h19	Transient Electromagnetic Exploration for Ground Water within Paleochannels of the North Eastern Goldfields, Western Australia	2	1100	269
Von Nagy-Felsobuki E I	**(Dept of Chemistry, University of Newcastle)**			
g19	Rovibrational Calculations of Helide Ions	4	3750	1885
Woodward C E	**(Department of Chemistry, University of NSW)**			
g87	Simulations of Nonuniform Polymer Fluids	2	4100	1463
Totals*			**34953**	**19307**

* Totals include projects not listed here which made little or no use of the grant