

## Computing and Networking Services

The primary mission of Computing and Networking Services (CaNS) is to provide the infrastructure and computing services within the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) for an advanced computing environment that enables staff, visitors, and collaborators to effectively use computer and network resources for their scientific and business requirements. In supporting growing business and research needs of EMSL in the area of information sciences, CaNS secures global information access to our facilities by providing online remote access to both computing resources and scientific equipment. A large portion of the efforts undertaken by CaNS staff members involves providing customer support to EMSL researchers and offsite users. For offsite users, CaNS provides secure information access and dissemination among EMSL researchers and a global scientific user community.

### Capabilities

One of the primary roles of CaNS is to provide computer support to all EMSL users and visitors, including scientists, technicians, and support staff. Computing support includes computer procurement assistance, setup, delivery, connection, and upgrade installation. System administration services include configuration management, software upgrades, security standards, account setup, and automated backup. CaNS is responsible for the design and implementation of EMSL's computing infrastructure, software, and Internet application development and support; conference room support; and management of computer maintenance contracts.

In Fiscal Year 2006, CaNS staff responded to approximately 6,600 formal requests for assistance (an increase of 20.6 percent over the 5,469 requests made in 2005) and 1500 informal requests. Demonstrating consistency and responsiveness, CaNS staff members resolve 50 percent of support requests within a day and 90

#### Expert Support and Services

- Security
- Desktop computing
- Scientific computing
- Instrument control systems
- Compute clusters and servers
- Infrastructure design and upgrade
- Web hosting and services
- Software application development and deployment
- Auditorium and conference room support

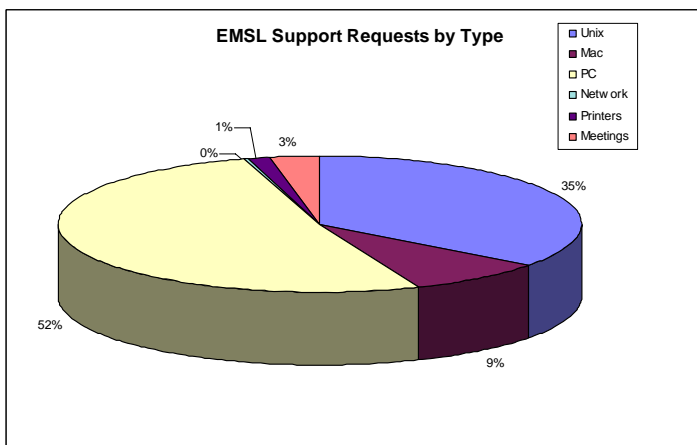


Figure 1. EMSL Support Requests by Type

percent within a week, giving priority to visiting scientists. Figure 1 shows a breakdown of computer support requests in 2006.

EMSL has a history of growth in the number and variety of computer systems used by its staff members (Figure 2). In Fiscal Year 2006, 361 systems were added to the support scope, and 177 systems were released, yielding a net increase of 184 systems (7.4%) and a total of 2023 systems in use in EMSL.

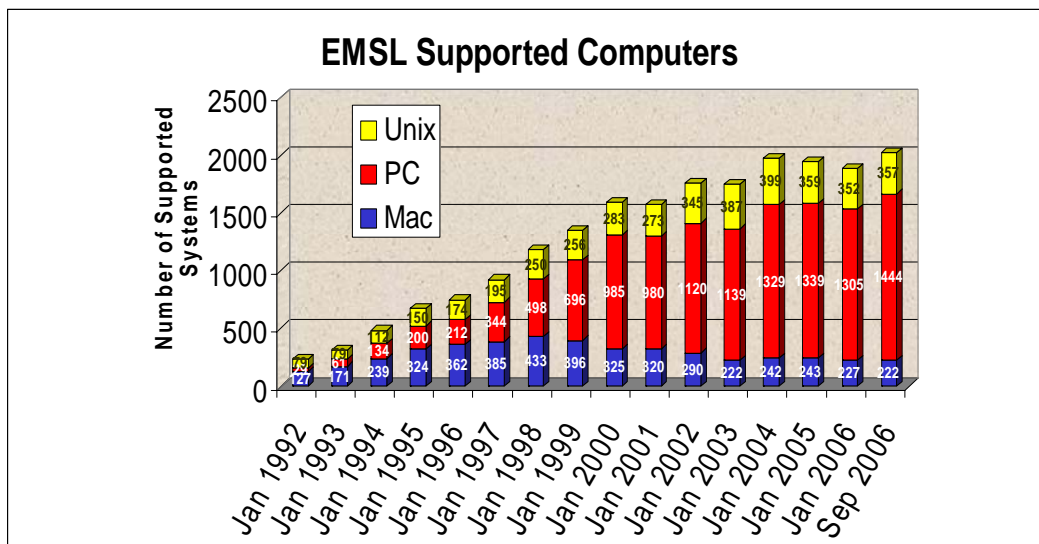
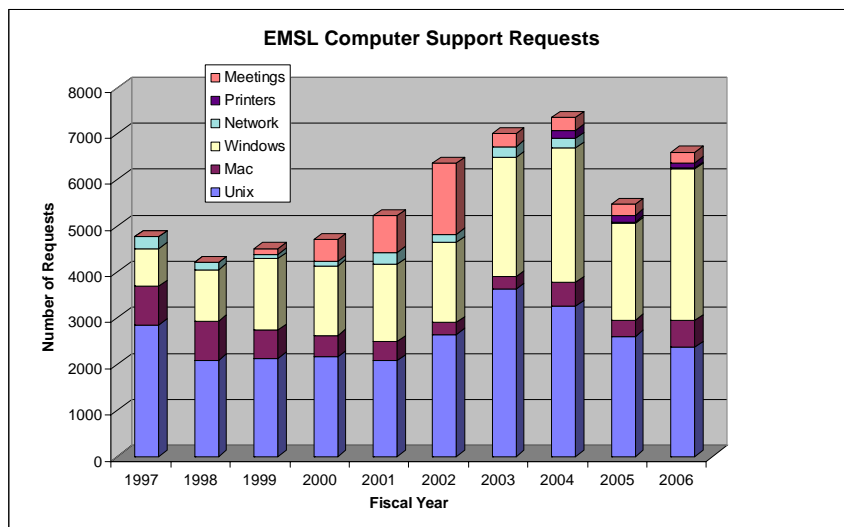


Figure 2. EMSL computer use trends.

In Fiscal Year 2006, CaNS added 163 new scientific users, increasing its support scope to 1043 active users. Of this total number of users, 564 use EMSL capabilities from offsite.

**Support Queues.** CaNS uses a web-based software-support request application (Footprints) to store and reply to submitted requests, and to record all dialogue surrounding problems. Users benefit by receiving a more thorough response, faster service, and an improved tracking system to ensure their problems are solved expeditiously. CaNS staff members benefit from the ability to better organize their work and identify chronic problems. CaNS also provides its support-request system to other projects in EMSL, such as NWChem and Ecce developers (see Molecular Science Computing Facility Overview section).

Data from Fiscal Year 2006 show that the 30 help queues were staffed by 116 administrators and experts, who together handled 15,000 support requests. Figure 3 shows historical use of the primary EMSL support queue, support@emsl.pnl.gov.



**Figure 3.** Computer support request history.

In 2005, an automatic support request satisfaction survey was implemented. Approximately one third of completed requests generate a survey query to the item's requestor. The requestor completes a simple survey rating our response and performance. The results are automatically recorded in a database and reviewed to identify areas for improvement. In Fiscal Year 2006, 308 customers replied. Average satisfaction with the service performed was 4.81 out of 5.0; average satisfaction with our response time was 4.81 out of 5.0. Six responses reported unsatisfactory service or response. These have been followed up on and corrective actions taken where necessary.

## Security

A major CaNS focus involves infrastructure and application upgrades designed to increase the security of EMSL's computing resources while continuing to provide open access for visitors and collaborators. This is an increasingly difficult task as new and more sophisticated security threats arise. Major project areas focused on the formation of the CaNS Cyber Security team. The focus of this team is to unify the efforts of the CaNS and MSCF cyber security teams, reduce redundancy, increase collaboration, and build greater trust and peer interaction between the projects. This team spans both server and client along with UNIX, Linux, PC and Macintosh platforms. Some of the security tasks that have come out of the formation of this team include development of a management network in the form of the Secure Collaborative Zone (SCZ), CaNS brown bags, expanded scanning for vulnerabilities, unified UNIX sign-on, and PointSec deployment.

**Secure Collaborative Zone (SCZ).** The SCZ is an internet accessible network for the purpose of allowing external collaborators access and storage of raw data files for experiments and analysis via web applications.

**Center for Internet Security Benchmarks.** Expansion of the Center for Internet Security (CIS) benchmarks was carried out for EMSL server infrastructure. CIS benchmarks enumerate security configuration settings and actions that "harden" systems. They are

unique, not because the settings and actions are unknown to any security specialist, but because consensus among hundreds of security professionals worldwide has defined these particular configurations. See <http://www.cisecurity.org/> for further detail. When vulnerabilities are detected from the scans, corrections are made in a timely manner due to the use of the EMSL support queue, to track and triage service requests. This expanded scanning assisted in EMSL's "outstanding" rating from the DOE Site Assist Visit auditors on network and system security.

**Unified UNIX sign-on.** In Fiscal Year 2006, work began to create a unified UNIX sign-on, providing users of PNNL resources the need to remember just a single user ID and password pair. Integrating UNIX authentications with PNNL Active Directory, thereby reducing UNIX password maintenance and auditing to that of the central AD service the lab already uses for Microsoft Windows based systems. Initial analysis has been completed, and several issues were identified.

**Tracking of security bulletins.** To better reduce duplication of effort, a CaNS Security Bulletin queue was established. This support queue is shared by all CaNS security task leads. Currently, the MSCF security task lead is responsible for triaging all incoming vendor and government (i.e., CIAC) cyber security bulletins and then determining to which platforms the notice applies, who is responsible for responding to the notice, and what action is needed. Previously, each security function within EMSL managed security bulletins autonomously. This centralized system greatly reduces and concentrates effort.

**Oracle upgrade.** EMSL-managed UNIX systems were patched for Oracle vulnerabilities. A primary application server was patched along with two other managed PNNL infrastructure systems.

**EMSL support queue server upgrade.** The EMSL support queue utilizing the Footprints software was upgraded. This migration entailed upgrading the physical server, the web server, the database engine, and the Footprints software. This web-based software is EMSL's primary mechanism for tracking, managing, and resolving all incidents and problems for both internal and external users. The upgrade was seamless to users and to the six support queues that rely on the software application to track issues.

**PointSec deployment.** CaNS Linux staff were instrumental in developing a Linux standard configuration. PointSec combines a required log in along with strong encryption (AES) to create an advanced security solution. When the user logs in, the laptop is unlocked and the single log in can also unlock the other tasks (e.g., operating systems, networks, PKI, or digital signing). PointSec:

- allows only authorized users to access information stored on mobile computing devices
- enforces automatic mobile security practices (i.e., transparent encryption)
- allows mobility without compromising security
- minimizes financial losses and mitigates legal and regulatory risks associated with exposing sensitive information.

**CaNS Brown Bags.** In Fiscal Year 2006, “CaNS Presents” was established as a monthly mechanism to share technical capabilities with EMSL users. The primary presenters are CaNS staff, though the presenters have come from across PNNL in an effort to exchange ideas, raise awareness and create a more secure computing infrastructure. Twelve presentations were given during Fiscal Year 2006 on topics ranging from configuring system administration tools such as kickstart to current trends in spam. All presentations were very well received, often standing room only. A complete listing can be found at <http://emslweb.emsl.pnl.gov/ops/comphelp/web/html/presentations.html>.

## Desktop Computing

**Windows/Macintosh Desktop Support.** The EMSL Office Computer Support team provided primary computer support services to more than 1300 Windows and 220 Macintosh computer systems. While the majority of these systems reside on user desktops, some systems are connected to specialized electronic instruments and devices that support the EMSL research mission. Most of the older Windows operating systems have been replaced with Windows XP and the Office 2003 suite, which provide EMSL users with increased reliability and capabilities, such as the ability to connect remotely to a desktop computer located in EMSL. Windows XP systems were upgraded to Service Pack 2 to implement needed security enhancements, and Software Update Service was implemented across the EMSL. Macintosh systems in EMSL are primarily G3, G4, and G5 models running OS X 10.4 and the Office 2004 suite.

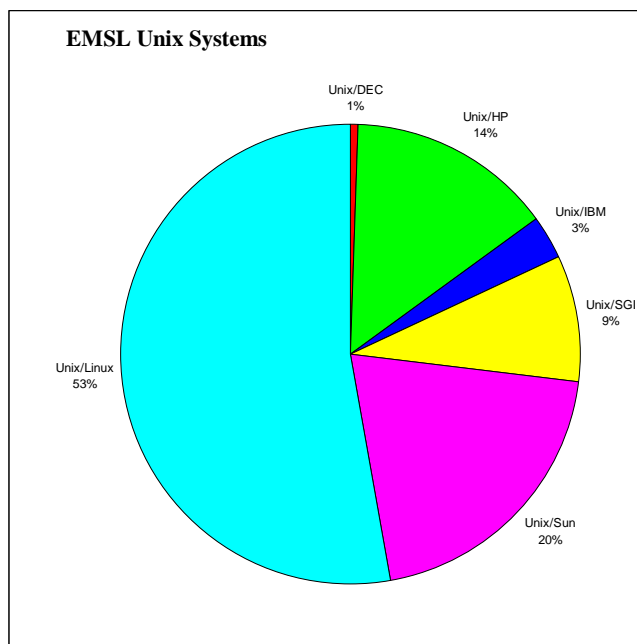
Along with numerous support requests from PC and Macintosh users for personal digital assistant support, wireless configurations, and remote access, the team responded to increased requests related to the EMSL enclave, including administration of SecurID tokens and EMSL domain accounts for non-staff members.

### Unix Desktop Support.

Linux continues to grow in popularity and is now the dominant Unix desktop operating system, increasing from a 47 percent share in 2005 to a 53 percent share in 2006 (Figure 4). We anticipate that Linux will continue to dominate the Unix desktop environment in the future.

With the increase in the use of Linux, an effort was made to standardize a Linux version, and 400 licenses were purchased for Red Hat Enterprise Linux (RHEL).

CaNS played a major role in the



**Figure 4.** Distribution of Unix operating systems.

testing and deployment of RHEL Linux, with team members maintaining the central Linux installation server. This new server allows EMSL staff members to easily install Linux and subscribe their system to an update service that automatically updates their computer when new operating system patches are released. The RHEL update service is analogous to the Microsoft Windows Update service.

## Scientific Computing

### Windows Scientific Computing Support.

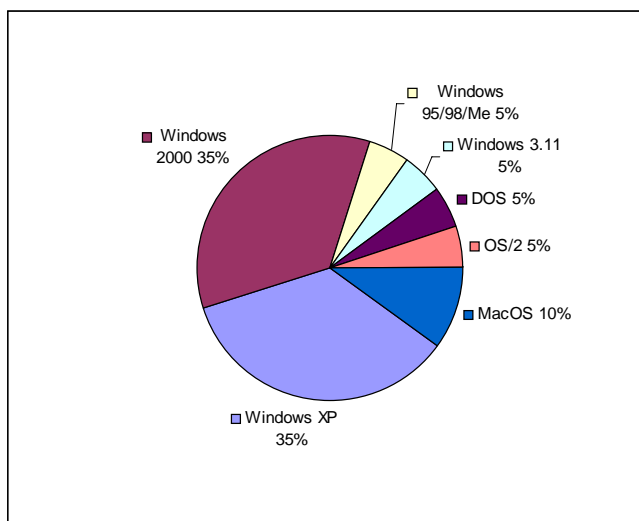
CaNS supports computers used to control scientific instruments during experiments or to collect data from experiments. A variety of Windows, Macintosh, and other operating systems are installed on these computers. The estimated distribution is detailed in Figure 5.

**Bionet** is the CaNS-created private instrumentation network that provides computer network connectivity between laboratories and storage resources. This network is isolated from the PNNL network connectivity

that is available in every office and laboratory, and it allows instrument control and data acquisition equipment to be connected to a network and available from specific gateways while protecting the equipment from all of the systems on the PNNL network. The number of machines on this network grew by 40 systems in Fiscal Year 2006 to a total of 125.

**Cluster Support.** A number of CaNS-supported Linux clusters experienced growth in both central processing unit (CPU) power and disk storage this year. The aging Weahltheow and Seattle clusters (64 CPUs total) were replaced by the Spokane cluster (with 74 new generation CPUs). In total, more than 20 terabytes of disk space and 64 CPUs were added to three Linux clusters. The number of supported Linux clusters is now 18, and they range in size from 8 to 200 CPUs. Customers continue to make extensive use of our test cluster, which now has both Gigabit Ethernet and Infiniband networking. Our test cluster also has the ability to run in either 32- or 64-bit modes, offering customers more options to test before deciding on a purchase.

The Math 1427 and ETB 104 computer rooms at PNNL were vacated this year. All cluster systems were relocated to the newly provisioned LSB 1C04 computer room.



**Figure 5.** Distribution of Windows/Macintosh operating systems installed on computers used to control research instruments or collect data (excluding office systems).

In 2006, we added four new clusters and one high-performance symmetric multi-processing system (SMP):

- Cam is a 16-node, 64-core cluster with 256 gigabytes of shared storage, a Myrinet high performance interconnect, and 32 gigabytes of total system memory (2 gigabyte per node).
- Spokane is an 18-node, 72-core cluster with 600 gigabytes of shared storage, a gigabit network interconnect, and 108 gigabytes of total system memory (6 gigabytes per node).
- Underlord is an 8 node, 32 core cluster with 900 gigabytes of shared storage, an Infiniband high performance interconnect, and 128 gigabytes of total system memory (16 gigabytes per node).
- Nwvisus (an existing 8 processor SGI system with 8 gigabytes of memory and a high performance video display subsystem) was replaced by a new 16 processor SGI with 32 gigabytes of system memory.

All of these clusters were procured through the PNNL Managed Hardware Program (MHP) where CaNS staff work with the MHP vendor to ensure availability of available components. The SGI system was procured with CaNS engineering/configuration participation.

CaNS continues to be the leader in cluster-computing solutions at PNNL.

**Supercomputing '05.** Tim Carlson managed the PNNL team that received the StorCloud challenge award at the Super Computing conference in Seattle in November 2005. The team consisted of scientists from EMSL and PNNL's Computational and Information Sciences Directorate, and corporate partners from HP, Cisco, and Federal Network Services. In addition to winning the StorCloud challenge, the team placed second in the Bandwidth challenge.

## Infrastructure Design and Upgrades

**Unix Infrastructure Backup System.** The EMSL disk-based infrastructure backup system continues to perform well. Its disk arrays were upgraded in capacity to 20 terabytes, and it provides for recovery of infrastructure and shared file system files for a one year window.

**Windows Server Backup Services.** The Windows Infrastructure Team replaced subscription backup services for its 40 Windows Servers with a Symantic BackupExec infrastructure. The PNNL subscription service moved to a model where cost varied with storage capacity, and a cost analysis indicated that it would be less expensive to provide a more robust system owned by the EMSL service center. All 40 of the managed servers were moved to this new model in Fiscal Year 2006.

**Unix/Linux Backup Services.** The desktop Unix/Linux team similarly began to replace subscription backup service for over 200 CaNS-managed Unix/Linux systems for the same reasons. A third of these systems have been relocated to a disk-based backup system built around the Amanda open-source backup software.

**Remote Installation Services (RIS).** The Windows Infrastructure Team deployed a Microsoft RIS server on the EMSL network that provides the ability to boot directly from the network and install an OS on systems that support pixie network boots. This is a core capability to enable the use of thin clients.

**Thin Client project:** CaNS funded a capability enhancement project to deploy thin client systems to utilize a Citrix-based Terminal Server to support 25 EMSL users or staff for their daily computing needs, thus eliminating their need for a full-sized, stand-alone desktop computer. There are several benefits to using this approach for desktop computing, the most visible being the reduced cost of hardware and maintenance. This project will continue into 2007.

**Distributed file services.** The CaNS strategy for high availability in its distributed file services (Andrew File System or AFS) configuration paid off several times in Fiscal Year 2006 as hardware component failures were repaired without disruption of service to users. Besides high availability, the EMSL distributed file system provides uniform access for users to their personal and project areas from any Windows, Macintosh, or Unix system; enhanced and secure file-sharing capability; consistent file backups; access to shared software; access to Website content; and consistent tools across platforms. Of the 3.5 terabytes of available space, 1.3 terabytes are in use, which leaves plenty of space for both transient files and long-term storage. Figure 6 shows the historical usage versus capacity.

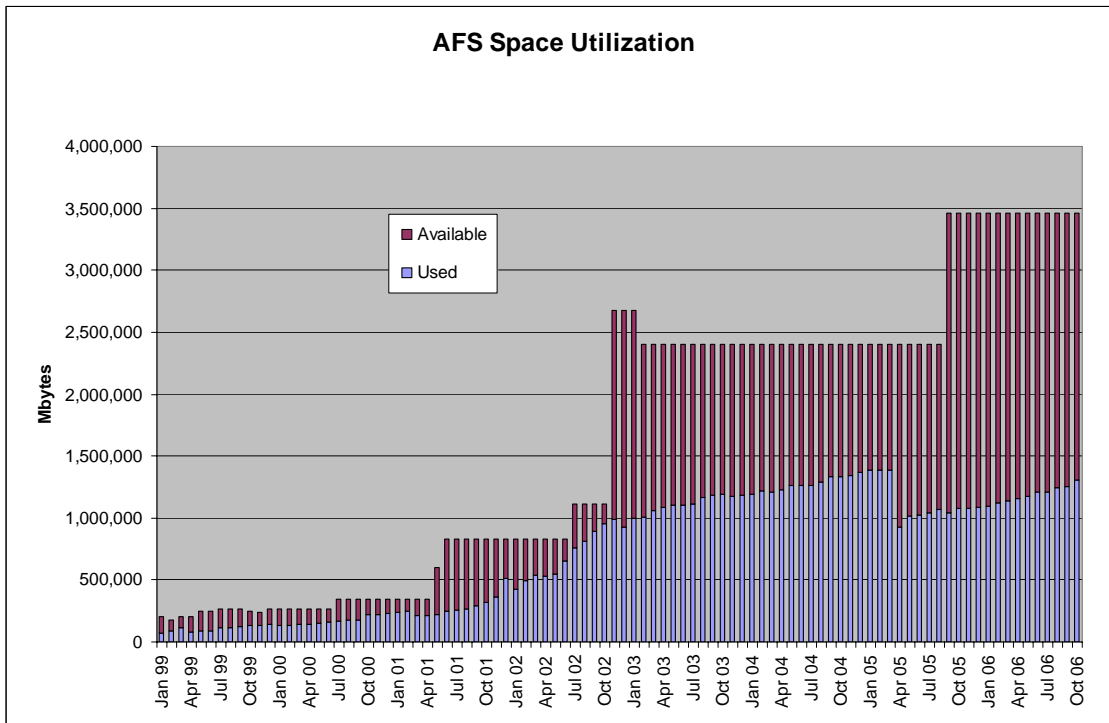


Figure 6. AFS capacity utilization.



## Web Hosting and Services

**EMSL Web Services.** Increased security concerns required EMSL to split its web server and move the server with external access to a more secure configuration. To accomplish this upgrade, the layout of the server configurations was redesigned, and the redesigned layout was implemented. A new server was purchased and deployed to house the external server, and the internal web server was moved to its own system. The external server was put behind proxy servers in 2005 to manage secure internal and external access. In Fiscal Year 2006, a second web server, linux based, was also deployed behind the proxy servers.

The EMSL Website continues to be moderately busy with about 1,109,000 visits in 2006. The Website absorbed almost 10 million hits during the year. Figure 7 shows the history of user visits.

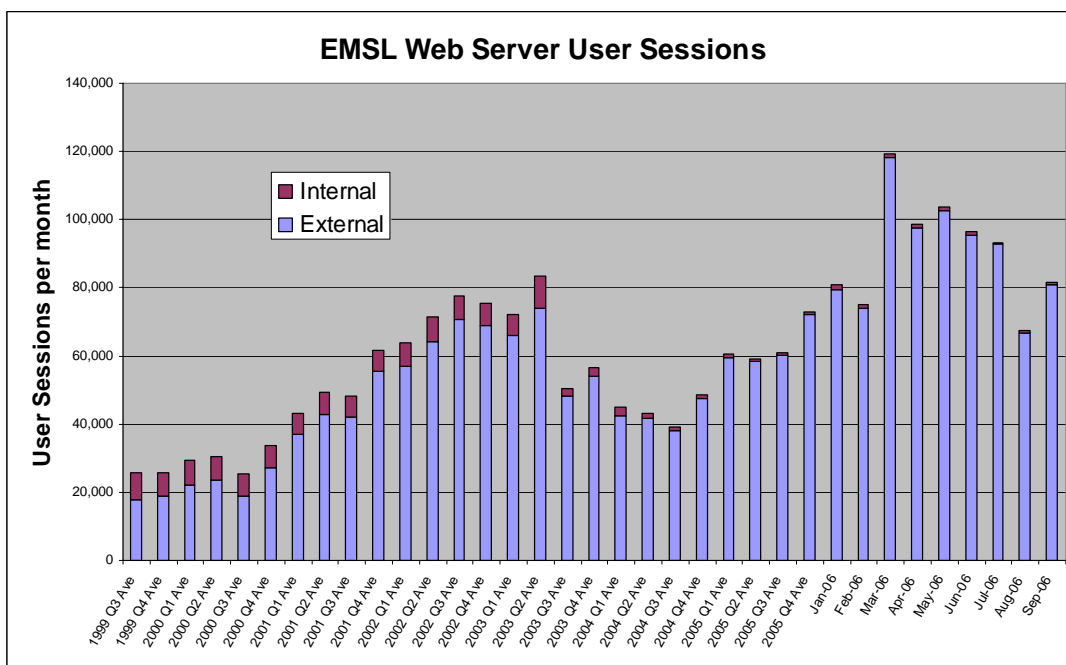


Figure 7. History of user visits.

## Software Application Development and Deployment

**Unix Software Repositories.** Software repositories provide shared access to frequently used software including freeware and floating license managers for commercial scientific applications. Applications in the repository include computer languages and interpreters; editors and debuggers; configuration management tools; documentation tools and pre-viewers; communication and collaborative tools; visualization, plotting, and graphing tools; numerical tools and libraries; data acquisition tools; and data management, structure, and format conversion. More than 150 applications available via this repository have been built and compiled to operate over the various operating systems that CaNS supports. The

repository is made available via the AFS distributed file system and provides the benefit of consistent applications that users do not have to build themselves.

## Auditorium and Conference Room Support

CaNS supported approximately 300 symposia, conferences, and meetings throughout the year. CaNS also worked in conjunction with Streaming Video Services to provide Internet Streaming for several meetings through the year, the “Director Lecture Series Seminars” being an example. These seminars put on by the PNNL Director’s Office host both PNNL and some external lecturers. The recorded meeting is hosted on the Director’s website for on-demand viewing.

CaNS staff are also working to upgrade equipment in the Battelle Auditorium. A new projector is on order along with some camera equipment. This will aid in video taping and live streaming from the Battelle Auditorium.

CaNS supported the following major events in Fiscal Year 2006:

- New Zealand visit
- Staff seminars and group meetings
- DOE Basic Energy Sciences Catalysis Initiative
- National Center for Research Resources Advisory Committee
- NMR Conference
- CH2M Hill Technical Exchange
- Actinide Conference
- PNNL Fundamental Science Directorate Review (Battelle Auditorium)
- Washington Round Table Board Meeting

## Future Directions

Funding was requested to support the Fiscal Year 2007 activities of CaNS.

- **Facility management.** Oversight, planning and management of the group.
- **Remote user support.** Direct support for users’ Unix accounts, including account creation and closure, password management, and file disposition.
- **Auditorium operations.** Technical support, supplies, and equipment for the EMSL auditorium and open conference rooms.
- **Expanded office support.** Expanded support for users and scientific instrument systems and EMSL staff directly supporting those users and systems. Deliverables, in

addition to those previously described, include delivery of network passwords to EMSL, support for the EMSL enclave, operating system and application software upgrades and security enhancements for Windows and MacOS, and access to mail and ETR without using SecurID.

- **Unix-based distributed file service.** Operation and management of EMSL's AFS distributed file system, which provides an independent platform, secure access to users' personal file space, shared project file space, and common applications. It also holds EMSL's web areas.
- **Windows based DFS and servers.** Windows user infrastructure including DFS space, user and project directories, some internal web space, mail and print servers, and terminal servers. It holds home directories for thin client users. Includes implementation and rollout of the EMSL thin client prototype, and, based on its acceptance, procurement of more clients.
- **Authentication services.** Operation and management of EMSL's authentication service providers. This includes completion of projects to consolidate authentication under PNNL's Active Directory service, development and implementation of account management policies and scripts, and background activities.
- **Email services.** Operation of EMSL's Unix email server, which provides routing of internal EMSL SMTP mail (generated on EMSL's Unix systems), routing of generic user mail from Unix to Exchange, and EMSL's mail list server.
- **Web application database services.** Operation of EMSL's database and application server, which provides back-end service for EMSL tours and user systems.
- **Security services.** Oversight of computer security issues for EMSL computing. This includes writing security plans, monitoring and responding to security bulletins, scanning EMSL systems, security training, configuration management, watching computer logs and responding to security situations, operating EMSL's Big Brother server, and other related activities.
- **Collaboratory service.** Support for EMSL-developed and -hosted Electronic Lab Notebook System, the virtual NMR, and other collaboratory services. The EMSL Collaboratory Support team assists in creating and supporting collaboration tools with EMSL that allow scientists the ability to access scientific instruments remotely and collaborate with others in a secure and effective manner.
- **Web-based help desk.** Operation of EMSL's web-based help desk system (Footprints), which currently hosts 30 support queues.
- **Web hosting services.** Support and operation of EMSL's web servers (internal and external), which host 11 external EMSL web sites including [www.emsl.pnl.gov](http://www.emsl.pnl.gov), [mscf.emsl.pnl.gov](http://mscf.emsl.pnl.gov) and six internal sites.

- **Core infrastructure operations.** This encompasses all activities that cannot be described in terms of services a user sees, but are required to make everything work. These include network management and operations, backup services, console server operation, license server operation, building and operating a test environment so things can be tested before they are put in service, implementation of maintenance contracts, computer facility management, and life cycle management. Approximately one quarter to one third of the infrastructure equipment should be replaced each year to keep the infrastructure operating efficiently and securely.

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