

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.

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

In 2005, CaNS staff members responded to approximately 5273 formal requests for assistance (a decrease of 21 percent over the 6715 requests made in 2004) and 1500 informal requests. Demonstrating consistency and responsiveness, CaNS staff members resolve 50 percent of support requests within a day and 90 percent within a week, giving priority to visiting scientists. Figure 1 shows a breakdown of computer support requests in 2005.

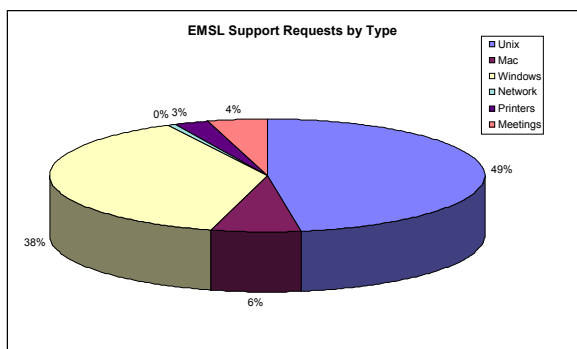


Figure 1. 2005 support requests by type.

EMSL has a history of growth in the number and variety of computer systems used by its staff members (Figure 2). In 2005, 301 systems were added to the support scope, and 352 systems were released, yielding a net decrease of 51 systems (2.7 percent) and a total of 1853 systems in use in EMSL.

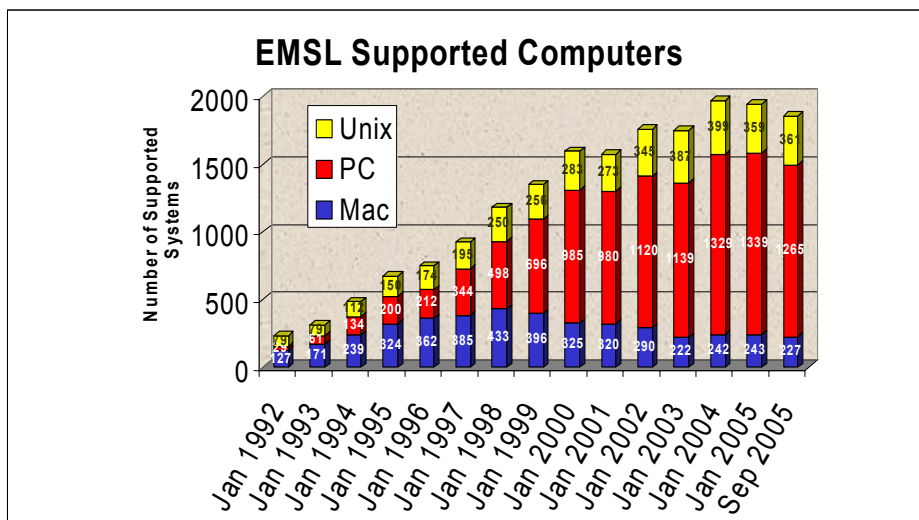


Figure 2. EMSL computer use trends.

In 2005, CaNS added 198 new scientific users, increasing its support scope to 1173 users. Of this total number of users, 621 use EMSL capabilities from offsite.

Support Queues. CaNS uses a software-support request application 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).

In 2004, a Web-based product called Footprints was installed to replace the EMSL Support Help Queue (ESHQ) request system, which had been developed internally and had become expensive to maintain. All 24 projects that used the ESHQ system were migrated to Footprints, and the ESHQ system was discontinued. This new system was upgraded in 2005 and now has 29 support queues.

Data from 2005 show that the 29 help queues were staffed by 115 administrators and experts, who together handled 14,500 support requests. Figure 3 shows historical use of the primary EMSL support queue, support@emsl.pnl.gov.

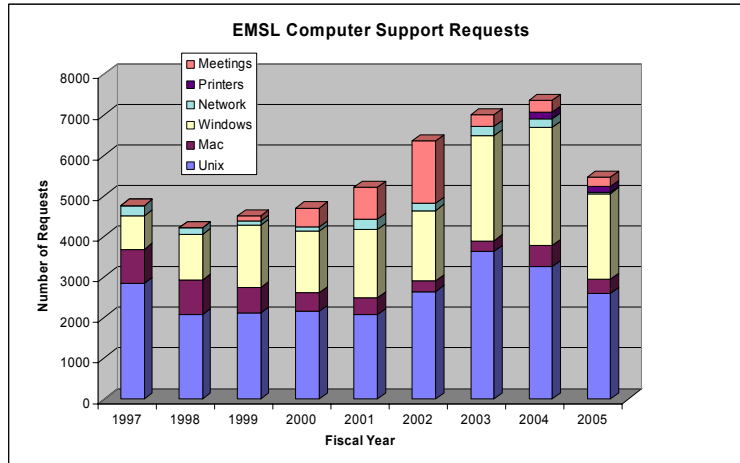


Figure 3. Computer support request history.

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. After implementation in mid-2005, 208 customers replied. Average satisfaction with the service performed was 4.76 out of 5.0; average satisfaction with our response time was 4.79 out of 5.0.

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 upgrade of SecureShell (ssh) access to include SecurID authentication and the continued evolution of the EMSL enclave as a network separate from the Pacific Northwest National Laboratory (PNNL) network. Smaller efforts involved eradication of inherently insecure protocols from our network, including telnet, ftp, rlogin, and earlier versions of ssh.

EMSL Enclave. To encourage open access while protecting PNNL from computational vulnerabilities, EMSL and PNNL implemented the EMSL enclave in 2004. EMSL enclave is a series of firewalls that isolate the EMSL computer network from the PNNL network and also from the open Internet.

A hierarchy of access requirements was implemented to provide the EMSL and PNNL networks with appropriate levels of security while protecting them from compromise. Thus, staff and users access the PNNL network remotely from their offices using methods similar to those that would be used to access the PNNL domain from home. Many staff connect daily using Virtual Private Network (VPN) software, which affords security by directing the user through a virtual tunnel into the network, and a SecurID code, which provides user authentication. The VPN software is uniquely configured as a half-tunnel to allow users to connect to the PNNL network simultaneously with the EMSL network.

To better enable data access across enclaves, a Windows-based distributed file system was implemented to provide users with access to shared data that are replicated on servers in two different buildings, thus providing reliability, backup, and disaster survivability. The new file share can be accessed from either the PNNL or EMSL enclaves without SecurID, thus solving a shared data access problem introduced by the EMSL enclave.

The enclave effort also included the development of separate services in the EMSL domain for non-staff, including EMSL visitors and students working in the facility. These groups were provided their own mail services and a terminal server (described below). They are able to access some PNNL services without the need for SecurID authentication.

The enclave implementation provided the foundation for easier access to EMSL by creating the framework for differentiating the EMSL and PNNL computer security requirements. The EMSL enclave implementation during 2004 was the result of a three-year effort involving multidisciplinary teams of staff from both EMSL and PNNL. Simplifying the use of VPN and enabling access to e-mail and additional Web/database applications without requiring a VPN connection were continuing enhancements made to the architecture in 2005.

SecureShell Remote Access. The ssh (ssh-gateway) access was completely re-engineered to support multiple enclaves and provide an enhanced level of security. Three new ssh-gateway servers that require SecurID authentication were deployed. SecurID provides a one-time-use authentication code that protects usernames and passwords from being compromised and then used to gain access to PNNL or EMSL systems. The three new ssh-gateway servers were deployed to both the PNNL and EMSL enclaves. Remote users that do not have a need to access PNNL resources can only use the EMSL gateway. Staff in the EMSL enclave, and remote-use staff and collaborators that require access to PNNL resources must use the PNNL ssh-gateway machine. Because almost all EMSL staff now carry and use SecurID to perform their daily work, CaNS capabilities have grown to include administration and management of SecurID tokens and their use for authenticating to the network.

Center for Internet Security Benchmarks. Implementation of the Center for Internet Security (CIS) benchmarks was accomplished 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. This set of security standards is being looked at by PNNL Computational & Information Sciences Directorate (CISD) across multiple platforms. EMSL/CaNS has opted to implement them now, as the standards are reasonable and soundly based.

Instrument Networks. In 2005, the System Update Service was expanded on the PNNL and EMSL networks. This service provides an automatic mechanism to apply security patches to Windows computers. The System Update Service, while ensuring security on Windows systems, is disruptive to scientific processes running on these systems as it can cause a system to reboot automatically, potentially causing loss of data on systems used to run experiments and collect data. Additionally, policy was changed to disallow

pre-Windows 2000 operating systems on the network because of security vulnerabilities in older Windows systems. Some software applications used to manage instruments or collect data are no longer supported by the vendor, making an operating system upgrade impractical on these systems.

CaNS implemented several instrument networks within EMSL to solve these problems. An instrument network separates a group of computers from the main network, and provides gateway computers connected to both the PNNL network and the isolated instrument network. The gateway computer provides access and file transfer capabilities to the instrument network. The legacy operating system computers are not on the main network, so they are not subject to operating system upgrade requirements.

Terminal Services. Terminal Services allows staff members to access common applications, such as Microsoft Outlook and Office applications, from a server rather than from their desktop. These servers are frequently used by staff members who do not have a Windows-based system available. There are several advantages to using Terminal Services.

- It eliminates the need for VPN running on the desktop.
- It allows access of e-mail and other applications from home using VPN.
- It allows access of e-mail and files from any computer.

EMSL Terminal Services was upgraded to better serve the EMSL community. CaNS currently operates four terminal servers that provide services to staff in the EMSL and PNNL enclaves, and to staff who connect remotely. Two of the terminal servers require SecurID authentication and are for users within the EMSL enclave. The third server provides regular access to users in the PNNL enclave. The fourth server is used by EMSL students and visitors and provides only the applications that these users can access.

Virtual Varian Nuclear Magnetic Resonance Gateway. The virtual Varian Nuclear Magnetic Resonance gateway was completely re-engineered and upgraded to use SecurID authentication for remote instrumentation control and to allow communication through encrypted ssh communications. This effort resulted in increased security, replacing clear-text passwords with encrypted authentication.

Sygate Rollout. CaNS staff members completed the roll-out of Sygate's Security Agent Software. This product is being implemented in EMSL to mitigate risk surrounding the use of the half-tunnel VPN connections from EMSL to PNNL and to allow the use of new remote access protocols, such as Grid computing. This year it was rolled out for use on all PNNL desktop computers and next year will be upgraded in EMSL. The Sygate Security Agent provides the following key security features:

- an application firewall that can permit or deny network traffic based on the application initiating the connection
- intrusion-prevention capabilities that detect malicious network traffic based on patterns observed in the traffic
- the application of different security policies based on the location of a system

- the ability to protect the system from revealing certain information about itself, such as browser type and operating system
- logging of security-related information.

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 newly formed EMSL enclave, including administration of SecurID tokens and EMSL domain accounts for non-staff members.

Enhancements were made to the VisitorLAN wireless network and management of visitor accounts on that network. Badged visitors are now given automatic accounts that allow access to the wireless network for the duration of their stay. Non-badged visitors who attend conferences and seminars in supported facilities also can gain access. CaNS manages a publicly available computer in the EMSL lobby that allows visitors to access the Internet and their e-mail accounts during their visits to EMSL.

Unix Desktop Support.

Linux continues to grow in popularity and is now the dominant Unix desktop operating system, increasing from a 35 percent share in 2003 to a 47 percent share in 2005 (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

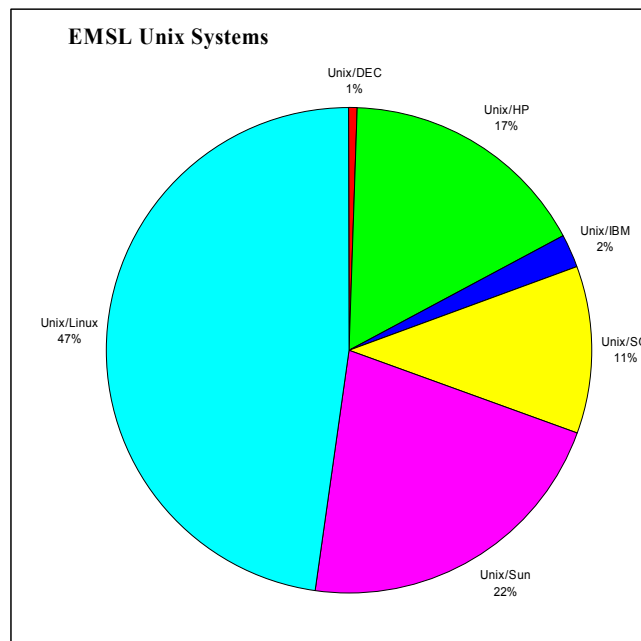


Figure 4. Distribution of Unix operating systems.

standardize a Linux version, and 400 licenses were purchased for Red Hat Enterprise Linux (RHEL). CaNS played a major role in the 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.

In 2004, CaNS developed and deployed a new patch and configuration management tool for Unix desktop operating systems. Previous configuration management and patching of supported systems was carried out by a set of custom-written scripts that were replaced in 2004 by an open-source tool called cfengine, which runs on all supported Unix systems. The CaNS team ported the legacy scripts to this new architecture with an emphasis on Linux. As a result, desktop machines are now automatically checked on an hourly basis for configuration file settings and security patches. In 2005, support for Solaris and Irix was added to this system.

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.

Data Storage Capability.

A 2-terabyte disk array was installed on the 11-t magnet to accommodate a data storage requirement in the High-Field Magnetic Resonance Facility.

CaNS staff researched, procured, and installed an eight-bay hard disk enclosure. The enclosure has a redundant disk configuration in case of drive failure. The project was a success, and we anticipate procuring and installing more of these arrays as data needs increase.

Clustering. A number of CaNS-supported Linux clusters experienced growth in both central processing unit (CPU) power and disk storage this year, including the Ransac, Aeolus, and Presidio. In total, more than 10 terabytes of disk space and 100 CPUs were added to three Linux clusters. The number of supported Linux clusters is now 16, and they range in size from 8 to 200 CPUs. Customers made extensive use of our test cluster, which now has

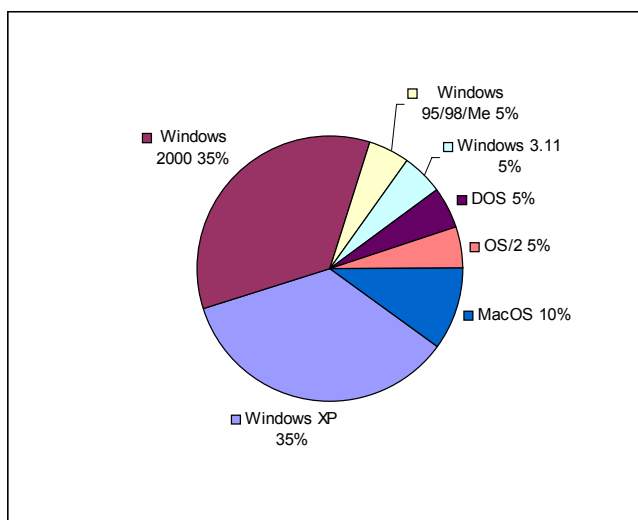


Figure 5. Distribution of Windows/Macintosh operating systems installed on computers used to control research instruments or collect data (excluding office systems).

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.

In 2005, we added three 64-bit clusters.

- Grapes is a 32-node, 64-CPU cluster; each node has 8 gigabytes of memory. The cluster uses both Gigabit Ethernet and Infiniband, and is used for capability development including the NWChem software package.
- CCN is a 16-node, 32-CPU cluster with a similar configuration. In this case each node has 6 gigabytes of memory and the access to 6 terabytes of shared storage. CCN is used for climate model development.
- ISC is a 14-node cluster for which we are currently testing both Lustre and Panasas file systems. ISC is designed to be a flexible cluster that can be configured in a number of ways to suit various projects dealing with network traffic analysis.

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

Infrastructure Design and Upgrades

Collaboration Enclave. EMSL funded a capability enhancement project to implement a secure collaboration zone (SCZ) in PNNL's OpenNet Enclave to provide high-performance connectivity that bypasses the PNNL central firewall complex. The SCZ project procured infrastructure servers, a network switch, and a prototype data-transfer system. Project staff developed a host-based security model in which the central firewall complex component was replaced by a centrally managed firewall on each Corporate Network Edition system. PNNL provided funding in 2005 to integrate the SCZ into the PNNL Enterprise Network Security Plan and to add in a hardware-based intrusion detection system. (This activity was a successfully completed CISC FY-05 PEMP goal). The SCZ methodology will be the primary high-performance network for collaboration with external networks and systems when its implementation is complete, allowing EMSL to take advantage of higher Internet bandwidth capabilities anticipated in 2006.

Wireless Upgrade. CaNS staff members, in collaboration with the Wireless Infrastructure Team, brought 802.11a and g wireless networking coverage to EMSL offices and conference rooms. This upgrade significantly increased available wireless bandwidth in EMSL, where the 11-Mbit 802.11b protocol was installed three years ago. This initial deployment and testing of the 802.11a wireless protocol is a precursor to a broader installation throughout PNNL. A wireless device must have 802.11a or g support to take advantage of the new service. The current implementation seamlessly switches among a, b, and g protocols.

Disk-Based Backup. The EMSL disk-based workstation backup system has been performing well. While this system has typically been used to back up Unix systems, the EMSL Windows servers are now also using this same disk-based backup.

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 2005 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. The AFS infrastructure was upgraded with new hardware and software, which increased its capacity to 3.5 terabytes. Of this available space, 1.2 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.

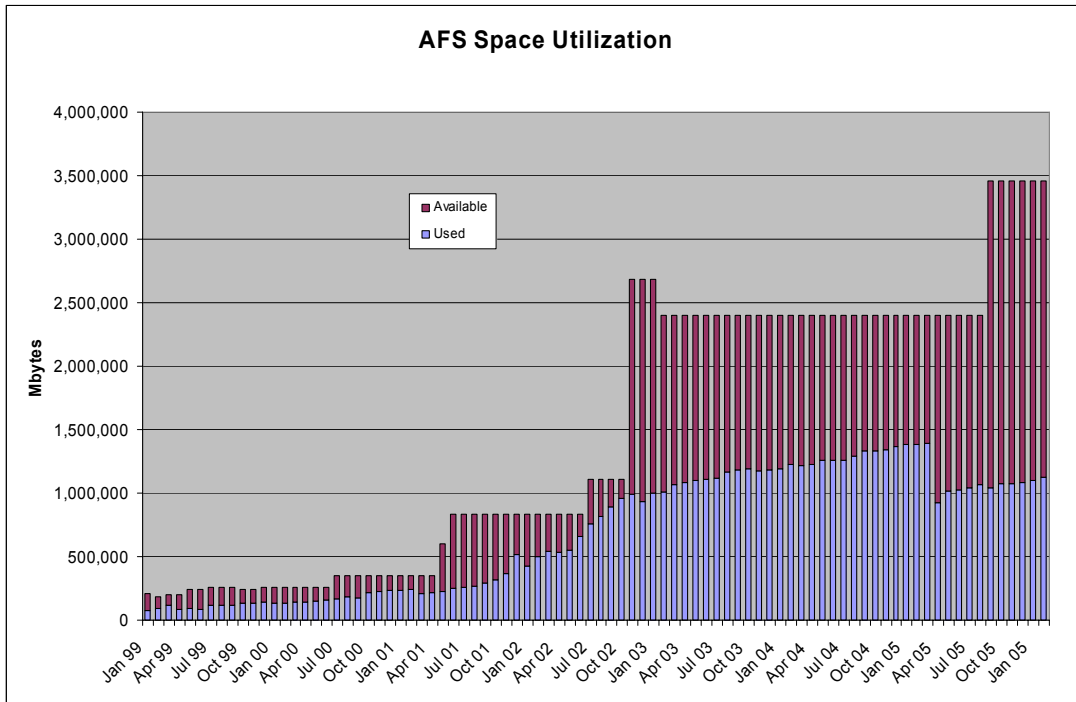


Figure 6. AFS capacity utilization.

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.

The EMSL Website continues to be moderately busy with about 675,000 visits in 2005. The Website absorbed over 10 million hits during the year. Figure 7 shows the history of user visits.

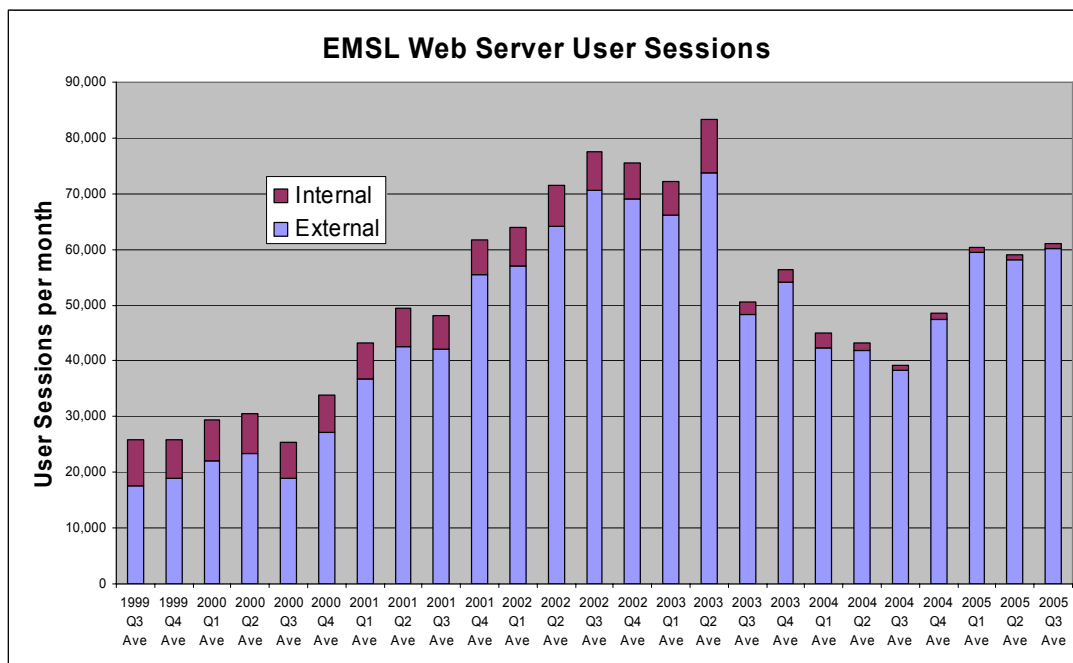


Figure 7. History of user visits.

Software Application Development and Deployment

EMSL User and Resource Systems (EUS and ERS). The EUS and ERS Web-based, work-flow tracking systems, which facilitate the use of EMSL resources, were significantly revamped in 2005. The user interface was overhauled and significant improvements were made on the underlying security of the host system and application. To meet security requirements, the system was moved behind the PNNL Netcontinuum systems in the Secure Web Zone.

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 253 symposia, conferences, and meetings throughout the year. With the help of an Internet media streaming server installed on the EMSL network

for electronic streaming of audiovisual presentations, EMSL streamed about a dozen live events, allowing offsite users to view these meetings in real time via the Internet.

The video cassette recorders in the EMSL Auditorium Booth were upgraded to updated hard drive video recorders and video home-system (VHS) digital video recorders. These new recorders give us the ability to create digital video disks (DVD) on the fly or from the internal hard disk in the hard drive video recorder unit. We also can convert from VHS format to DVD format. These new units are installed in the rack and wired into all the main components of the EMSL auditorium. The final cut edit station was wired in the main rack. This gives the ability to transfer information from video tapes or captured files from the edit station of past meetings to the DVD recorder for archiving on DVD. We then reuse the tapes, thus realizing \$6 to \$30 each over the cost of new tapes.

A new projector was procured for the auditorium. It provides improved display capabilities and allows the old projector to serve as a backup.

CaNS supported the following major events in 2005:

- a Russian delegation
- staff seminars and group meetings
- HPCS3 Greenbook Workshop
- Hanford Natural Resources Trustee Council onsite briefing
- Battelle Laboratories Cyber Security meeting
- The EMSL onsite review
- EMSL Laboratory Advisory Committee meeting
- Computational Science and Engineering Initiative Advisory Committee meeting
- Congresswoman Cathy McMorris visit.

Future Directions

The CaNS group will continue to support staff and users within established Service Level Agreements. All desktop computing systems, IT infrastructure, and audio/video capabilities require continued effort to maintain them at an operational, secure, and compliant level. Anticipated activities are identified below.

- Refinement of the EMSL Enclave operating environment will continue with additional Web and database services being deployed to the exonic splicing enhancers and development of a Web-based time reporting system.
- Operating system upgrades and security enhancements will continue.
- Microsoft Office application upgrades and security enhancements will continue, including rollout of the new Microsoft Windows operating system, Sygate upgrade, and new Norton virus-checking software.
- An ssh upgrade will occur for remote access to Unix systems.

- Distributed file system upgrades will occur, including moving to new software with improved performance capabilities.
- The collaboration network infrastructure, procured in fiscal year 2004 and tested in fiscal year 2005, will be released for general use. This network infrastructure enhancement will allow high-performance data transfer between PNNL and collaborators.
- The storage area network (SAN) infrastructure procured in fiscal year 2005 will be deployed to directly link the EMSL SAN with the PNNL SAN.
- Operations, support, and enhancement of the auditorium and conference room capabilities will continue.
- The CIS benchmarks will be deployed to desktop Solaris and Linux systems.

Staff

Linda M. Connell, Technical Lead
(509) 376-2375, linda.connell@pnl.gov

Kevin M. Regimbal, Technical Lead
(509) 376-2246, Kevin.Regimbal@pnl.gov

Tracy M. Loew, Administrator
(509) 376-1211, tracy.loew@pnl.gov

Scott W. Campbell, IT Specialist
(509) 376-2952, scott.campbell@pnl.gov

Timothy S. Carlson, Senior Research Scientist
(509) 376-3423, timothy.carlson@pnl.gov

Boyd L. Champion, IT Specialist
(509) 376-2287, boyd.champion@pnl.gov

Patricia M. (Shelly) Fangman, Research Scientist
(509) 376-5382, shelly@pnl.gov

Phillip P. Gackle, Senior Research Scientist
(509) 375-2130, philip.gackle@pnl.gov

Dan N. Hagedorn, Senior Research Scientist
(509) 376-8206, dan.hagedorn@pnl.gov

Zoë C. Johns, Research Scientist
(509) 376-2038, zoe.johns@pnl.gov

Bryce P. Kaspar, IT Specialist
(509) 376-3949, bryce.kaspar@pnl.gov

Jeffrey Larsen, IT Specialist
(509) 376-1729, jeff.larsen@pnl.gov

Tim J. Lawson, Research Scientist
(509) 376-2137, timothy.lawson@pnl.gov

Thomas J. Mathieu, User Support Coordinator, Senior Research Scientist
(509) 376-9711, tom.mathieu@pnl.gov

Nicholas A. Nanni, Technician
(509) 376-1714, nick.nanni@pnl.gov

Douglas J. Nordwall, Senior Research Scientist
(509) 376-4308, doug@pnl.gov

Shaun T. O'Leary, Senior Research Scientist
(509) 376-3505, shaun@pnl.gov

Andrew E. Rakowski, Senior Research Scientist
(509) 375-2238, landrew@pnl.gov

Michael S. Russcher, IT Specialist
(509) 376-0300, mike.russcher@pnl.gov

Aaron I. Thronas, Research Scientist
(509) 376-1170, aaron.thronas@pnl.gov

Tyson A. Tucker, Student
(509) 528-8169, tyson@pnl.gov

Ralph S. Wescott, Senior Research Scientist
(509) 372-6901, ralph.wescott@pnl.gov

Cheryl A. Wilmoth, IT Specialist
(509) 376-2327, cheryl.hartwell@pnl.gov

Matrixed Staff

Gerald A. Funnell, Electrician
(509) 372-6276, gerald.funnell@pnl.gov

Paul D. Gjefle, Senior Research Scientist
(509)375-2528, paul.gjefle@pnl.gov

Bruce J. Herrin, Electrician
(509) 376-0512, bruce.herrin@pnl.gov