

Computer and Network Services (CaNS)

The primary mission of the CaNS Group is to provide the infrastructure and computing services within the W.R. Wiley Environmental Sciences Laboratory (EMSL) for an advanced computing environment that enables staff, visitors, and collaborators to effectively use computer and network resources for their scientific research and business requirements. In supporting EMSL's growing business and research needs regarding 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 CaNS Group's efforts 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

CaNS staff provide complete computer support for all EMSL computers including PC, Macintosh, and UNIX systems. CaNS provides computer procurement assistance, setup, delivery, connection, upgrade installation, and 24-hour computer emergency support. 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 2003, the CaNS staff responded to approximately 7000 formal requests for assistance and to an estimated 1500 informal requests. Conference room support and multimedia services reflect significantly growing areas this year with the expansion of our external user base. Demonstrating consistency and responsiveness, CaNS staff resolve 50% of support requests within a day and 90% within a week, giving priority to visiting scientists.

Figure 1 shows a breakdown of computer support requests in 2003 by platform.

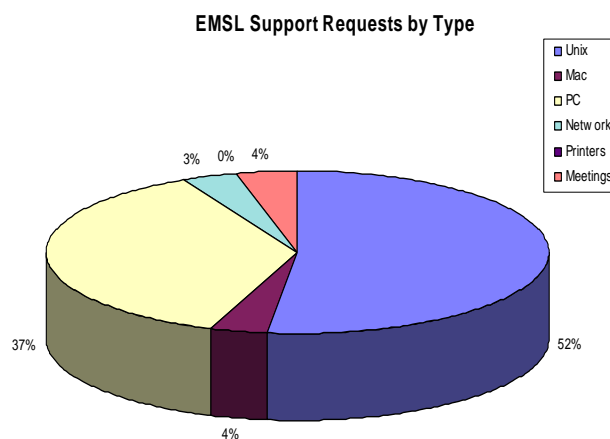


Figure 1. Calendar year 2003 support requests by type.

EMSL has a long history of growth in the number and variety of computer systems. New challenges are anticipated in the areas of personal digital assistants (PDAs) and wireless systems, and in the number of computer systems supported by remote users of the facility. The chart in Figure 2 illustrates this historical growth in computer use. In 2003, 419 systems were added to the support scope and 197 systems were released, yielding a net increase of 222 systems (12.7%) to a total of 1970 systems.

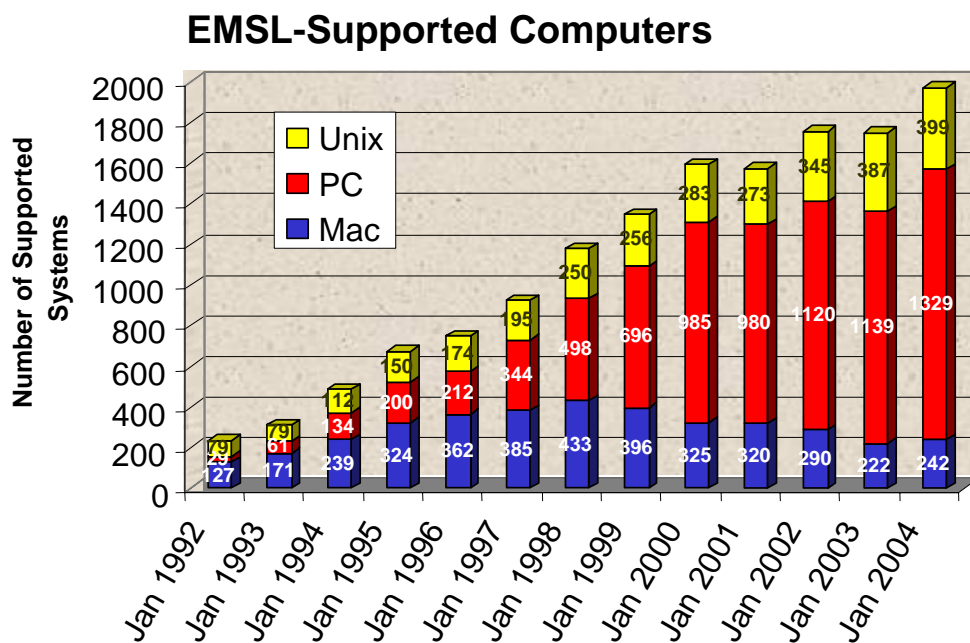


Figure 2. Historical growth in computer use.

In 2003, CaNS added 263 new scientific users to bring its support scope to 835 users. Of these users, 372 are remote users.

Office Computing & Conference Room Support

Desktop Computer Support. EMSL's Office Computer Support team provided primary computer support services to EMSL's more than 1250 PC and 220 Macintosh computer systems. While the majority of these systems reside on user desktops, some systems are connected to EMSL's specialized electronic instruments and devices in support of the research mission. In addition to satisfying the daily support requests from PC and Macintosh users, the team responded to an increasing number of support requests for PDAs, wireless configurations, and remote computers.

While older Microsoft operating systems are being retired, the number of PCs upgrading to Windows XP increased significantly. The new operating system (OS) provides EMSL users with increased capability and reliability. The more than 220 Macintosh systems in EMSL are mostly G3 and G4 models running MacOS 9.x/OS-X and the Office X suite. Many of these systems were upgraded to OS-X throughout the year.

Windows Servers. To facilitate day-to-day office computer users, several strategies were implemented. Licensed servers provide access to common desktop applications for Macintosh and PC systems throughout the facility at a reduced overall cost. Automated PNNL network installers are available (to staff) for a range of commercial and locally developed software including word processing, spreadsheets, drawing, and presentation

applications; scientific graphics; project management; relational databases; equation manipulation and solution; viewers for documents and Pacific Northwest National Laboratory (PNNL) databases; and user clients for PNNL applications.

Conference Room Support. An IMS5 Internet media streaming server was installed on the EMSL network for electronic streaming of audiovisual presentations. This dedicated EMSL server allows off-site users to view meetings in real time via the Internet.

Infrastructure

EMSL Enclave. The term “enclave” refers to a division of a network into separate zones with communication across firewalls. The EMSL enclave was developed after visitors (often from non-U.S. countries) obliged us to evaluate our network security strategy. It is anticipated that future enclaves will be established, further separating networks with higher security needs from those with lower security needs. As network security tightens, separating EMSL from the PNNL network hopefully will exempt EMSL from some of these tighter controls. The primary initial impact on users in this multiple enclave configuration will be that access from a more open enclave (e.g., EMSL) to a less open enclave (e.g., PNNL) will require the use of SecureID authentication (also known as a “smartcard”).

Equipment needed for this conversion was purchased and partially deployed this past year. Final testing, evaluation of configuration alternatives, and conversion of applications is ongoing and expected to be completed in March 2004.

Windows Instrument Network. This year, Windows 95 and Windows NT-based computers became prohibited on the PNNL network because Microsoft was no longer providing patches and updates, thus making these operating systems insecure. However, a significant number of EMSL instruments are connected to these older computers, which could not be upgraded because of hardware or software incompatibilities. CaNS staff resolved this dilemma with the creation of an “Instrument Network.” The older computers were equipped with two network adapters to connect to both a private network (connecting one or more instrument computers) and to the EMSL network. A common file share was made available to both the instrument computers and office computers with EMSL network access, thus allowing the sharing of data between the two networks.

Gigabit Capability. CaNS staff deployed copper gigabit capability in EMSL to support both office and scientific computing. The first phase was completed in August with more than 40 computers benefiting from the installation of gigabit switches in office and laboratory areas. The EMSL core network was also extended to a multidisciplinary computational laboratory providing 48 ports of gigabit copper to this growing computer facility. The Molecular Science Computing Facility (MSCF) received an additional 48 ports at the end of the fiscal year.

Disk-Based Backup. EMSL’s workstation backup and restore tape-based backup system was replaced with a disk-based storage system expected to be 10 times faster. Besides improving performance, the new system will avoid the risk of tape read errors and failures and provide faster restore capabilities.

Extranet Services. New infrastructure racks were installed to give EMSL the ability to extend services to the PNNL extranets. This new infrastructure will be useful for offsite backups and to locate some redundant services in support of the new enclave model. The EMSL web server housing the external EMSL website will be moved to the extranet in 2004.

Distributed File Services. The CaNS strategy for high availability in its distributed file services (Andrew File System or AFS) configuration paid off several times this year 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 EMSL Unix or PC system, enhanced and secure file-sharing capability, consistent file backups, access to shared software (described later), access to maintain web pages, and consistent tools across platforms. Of the 2.4 terabytes of available space, 1.2 terabytes are in use, which leaves plenty of space for both transient files and long-term storage. Figure 3 shows the historical usage versus capacity.

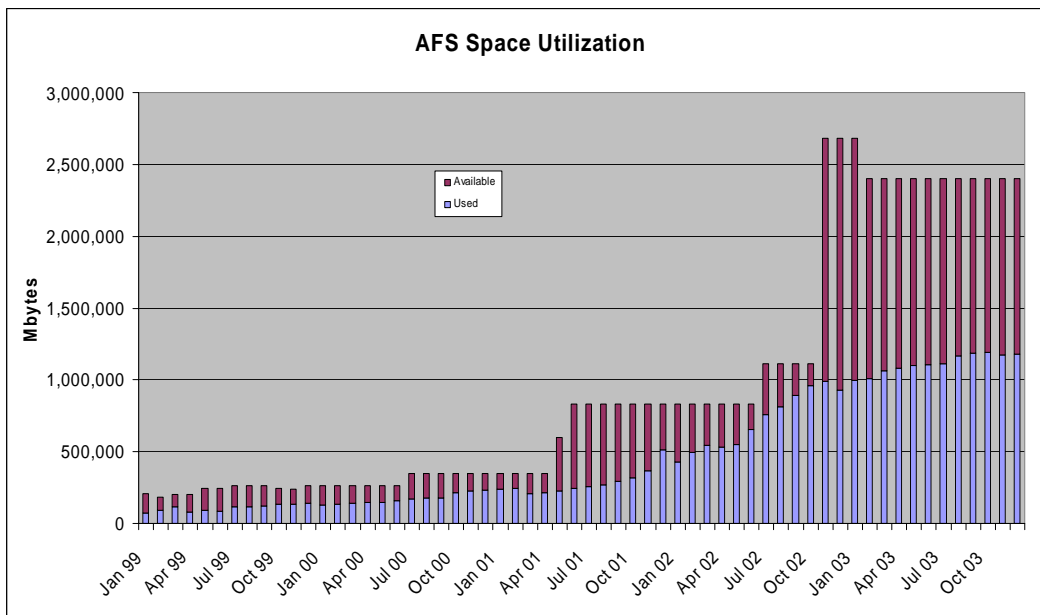


Figure 3. AFS capacity utilization.

In addition, the OS on servers in the infrastructure was upgraded to the latest version, and more rack-mountable systems were installed to replace older models. This enabled us to consolidate several cabinets into two and make room for the new supercomputer.

Application and Web Services

EMSL Web Services. Increased security concerns will require EMSL to split its web server and move the server with external access outside the PNNL firewall. To accomplish this, the layout of the server configurations was redesigned and deployed. Also, a new server was purchased to house the external server. A few issues remain to be resolved early in 2004. Once these are resolved, the EMSL web services will be split, and the external server will be put on extranet (an intranet that is partially accessible to authorized outsiders).

The EMSL website continues to be moderately busy with about 790,000 visits in 2003 (up 1.1% from the prior year). The website absorbed 21 million hits during the year. Figure 4 shows the history of user visits.

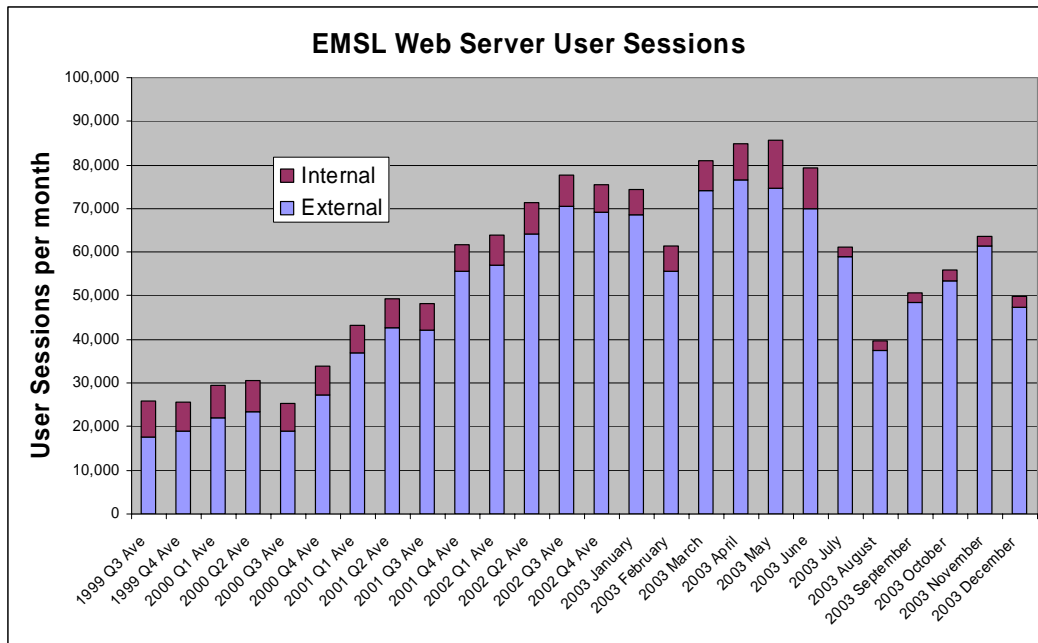


Figure 4. History of user visits.

Support Queues. One of the primary roles of the EMSL CaNS group is to provide computer support to all EMSL users including scientists, technicians, and support staff. The most commonly used method to report a problem is via email and web forms. Software enables CaNS staff to store the submitted email requests and to access and reply to them, and record all dialogue surrounding the problem. Users benefit by receiving a more thorough response, faster service, and an improved tracking system to ensure their problems are solved expediently. CaNS staff benefit from the ability to better organize their work and identify chronic problems.

The EMSL Support and Help Queue system was developed in EMSL and deployed by CaNS in 1999 to provide this service. This year, the cost of maintaining the system became prohibitive, and a project was undertaken to identify a commercially supported package to provide this service more effectively. After looking at several options, a web-based product called Footprints was installed in July, and the primary CaNS support queues were converted to use it. The remaining EMSL queues will be migrated in 2004.

Data from 2003 show that the 26 help queues were staffed by more than 130 administrators and experts, who together handled 14,500 requests for help and support from EMSL staff and users. Figure 5 shows historical use of the primary EMSL support queue, support@emsl.pnl.gov. The growth in requests in 2003 was 10%.

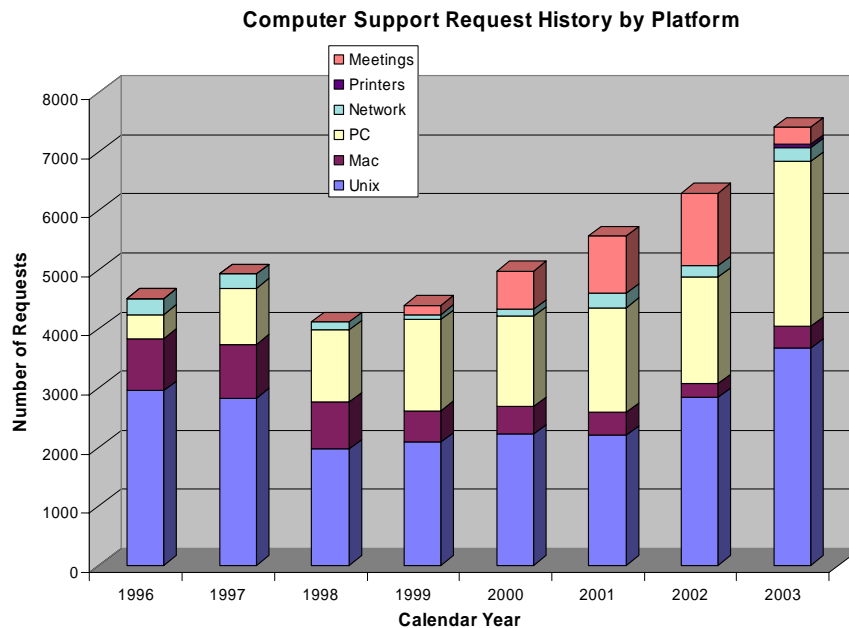


Figure 5. Computer support request history.

EMSL Resource System (ERS). The ERS web-based tool was developed to track usage of EMSL's major instruments and facilities. The design and development of ERS began in 2002. In 2003 all facilities started tracking major instrument usage. An algorithm for defining usage of the large variety of instruments tracked in the ERS was established, and the system was enhanced to be able to generate reports that break down quarterly or annual usage by usage type.

The ERS was also upgraded to import data directly from nine of the spectrometers in the High Performance Mass Spectrometry Facility. Information about samples run on the mass spectrometers is entered into the Data Management System and stored in a database. The ERS imports this information into its own database nightly, thus avoiding duplicate data entry by the spectrometer custodians in both systems.

EMSL User System (EUS). The EUS web-based work-flow tracking system facilitates the use of EMSL, starting from the initial request for use of EMSL resources to the tracking of publications resulting from each use. The EUS was implemented on October 1, 2002. In 2003, the system was enhanced to include complete tracking of MSCF software products such as NWChem and Ecce. It also has been enhanced to support all aspects of requesting and tracking agreement forms, such as Non-Proprietary Use Agreements. New administrative pages allow management of users, institutions, and instruments in the database. The EUS now includes 40 reports that allow EMSL to track statistics on users, their professions and institutions, areas of science, funding sources, etc.

Scientific Computing and Unix Desktop

Unix system support continued this past year for CaNS. We still support five OS, Redhat Linux, Sun Solaris, SGI IRIX, HP-UX, and IBM AIX (ordered from the most common

OS type to the least used). We now support more Linux systems than any other OS. Figure 6 shows the distribution of Unix operating systems.

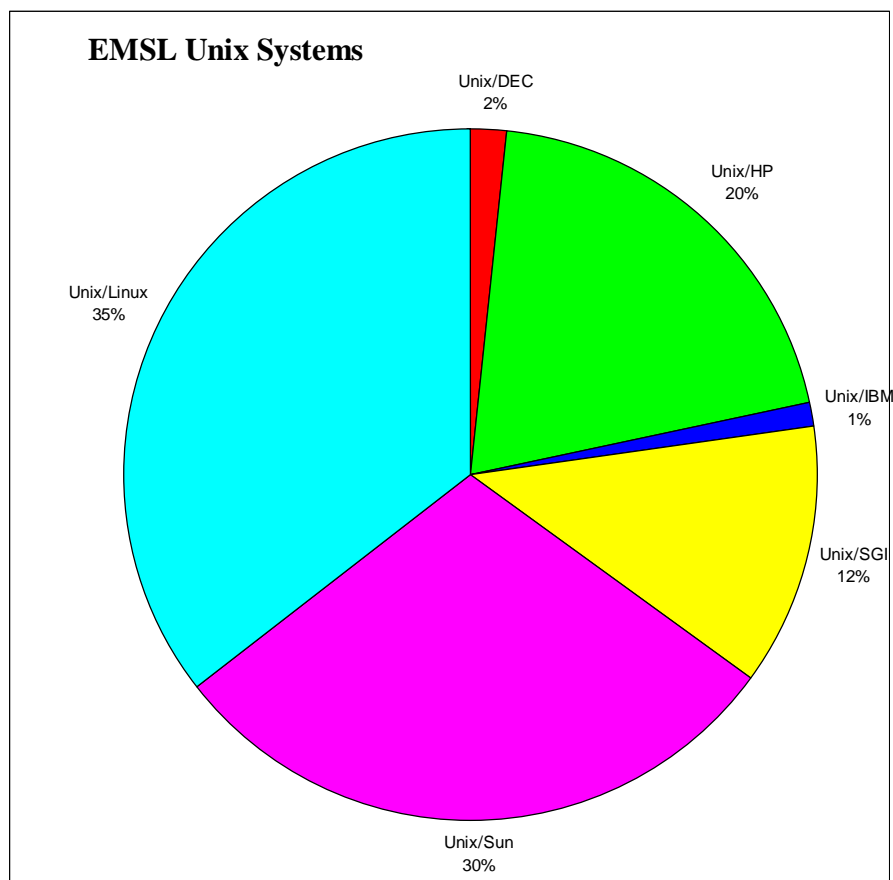


Figure 6. Distribution of Unix OSs.

Upgrades and security patches are continually required in the support model for CaNS to provide capability enhancements, support new hardware, and plug security holes. EMSL Unix desktop, infrastructure, and computational systems were upgraded to the latest OS, application services, and security patches to meet security operations mandates. This work was done with scripts and automated procedures the team developed to implement the standard EMSL configuration on all machines remotely. This standard configuration facilitates support of user systems and minimizes unavailability of systems to their users.

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 are available via this repository and have been built/compiled to operate over the various OS flavors. The repository is made available via AFS, our distributed file system and provides the benefit of consistent applications that users do not have to build themselves.

Clustering. Clustering technologies and methodologies coupled with the adoption of Gigabit-Ethernet as the PNNL network backbone have brought about many opportunities for experimenting with high-bandwidth networking and multi-node computational solutions for our customers. We are currently managing 15 Linux clusters that vary in size from 8 to 160 processors each. In keeping with current technology trends, the Unix Scientific Computer Support team upgraded its testbed cluster to an 8-processor (2.4 GHz Xeon, 4 node) cluster with fast Ethernet, Gigabit Ethernet, and Myrinet network backplanes, thereby allowing scientists to experiment and benchmark before they buy their own hardware.

Staff

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

Cheryl E. Hall, Administrative Secretary
(509) 376-2499, cheryl.hall@pnl.gov

Scott W. Campbell, Senior 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, Research Scientist
(509) 375-2130, philip.gackle@pnl.gov

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

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

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

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

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

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

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

Douglas J. Nordwall, 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

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

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

Matrixed Staff

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

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

Students

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

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

Julie R. Wiganosky, Student
(509) 376-2129, julie.wiganosky@pnl.gov