William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

Environmental Molecular Sciences Laboratory Operations Manual

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Office of Science
U.S. DEPARTMENT OF ENERGY

Acronyms

CAT	Collaborative Access Team
DOE	U.S. Department of Energy
EMSL	William R. Wiley Environmental Molecular Sciences Laboratory
EPR	electron paramagnetic resonance
ERICA	Electronic Records and Information Capture Architecture
ES&H	environment, safety and health
IOPS	Integrated Operations System
NMR	nuclear magnetic resonance
PNNL	Pacific Northwest National Laboratory

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1.0 Introduction

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a state-of-the-art user research facility supported by the U.S. Department of Energy's (DOE's) Office of Biological and Environmental Research and operated by the Pacific Northwest National Laboratory (PNNL). This handbook provides the framework for achieving EMSL's vision of excellence as a model scientific user facility; it is also aligned with the fundamental mission of DOE's Office of Science to advance basic research and develop the tools of science that comprise the foundations for the applied missions of DOE and PNNL.

This handbook is organized by sections that describe EMSL's operational aspects:

- Section 2 describes EMSL's mission, vision, and core values.
- Section 3 describes EMSL's management and advisory committees.
- Section 4 provides an overview of EMSL's facilities and supporting capabilities.
- Section 5 describes the methods by which users may access and use EMSL resources.
- Section 6 describes the tools to facilitate user services such as training, security, and tracking.
- Section 7 describes EMSL's budget allocations, charging guidelines, and space use.

2.0 EMSL Mission, Vision, and Core Values

2.1 Mission

The mission of EMSL as a national scientific user facility is to create an integrated environment for scientific discovery and technological innovation in pursuit of the nation's most difficult and critical challenges by:

- Providing advanced instrumentation and computational resources to scientists engaged in research of the physical, chemical, and biological processes that underpin environmental and other critical scientific issues to meet the missions of DOE
- Providing a model for interdisciplinary scientific teams, bringing an integrated set of capabilities to bear on a complex scientific problem
- Educating students and scientists in areas of molecular science to meet the demanding multidisciplinary challenges of the future.

2.2 Vision

The vision of EMSL is to be DOE's premier user facility for solving complex problems by addressing a diverse set of scientific challenges. As such, EMSL will be recognized as:

- A valued strategic partner to other institutions and individuals pursuing fundamental investigations in molecular and computational science
- A leader in the development of science-based solutions applicable to environmental remediation and restoration of the DOE complex and other environmental stewardship issues
- A leader in developing, applying, and providing advanced scientific tools to the scientific community for expanding scientific frontiers.

EMSL's success reflects the commitment to three signature characteristics as a national user facility:

1. Highly competent research teams who develop enhanced research tools and methodologies that advance EMSL capabilities.
2. Integration of theory, modeling, and simulation with experimental programs when appropriate.
3. A collaborative mode of operation leading to joint publications and enhancement of research programs at user institutions as well as at EMSL, effectively leveraging DOE's investment in this facility.

2.3 Core Values

Staff, customers, users, and collaborators hold EMSL in high esteem because of its commitment to the following core values:

- Teamwork: A commitment to work in collaborative teams.
- Integrity: A commitment to the highest professional standards for excellence.
- Impact: A commitment to address significant scientific challenges that address major societal needs.
- Creativity: A commitment to intellectual leadership contributing to scientific and technical problems and a commitment to staff to provide an atmosphere that encourages and fosters creativity.
- Objectivity: A commitment to provide to the scientific community and the nation unbiased scientific results and solutions based on scientific data rather than opinion.

3.0 EMSL Management and Advisory Committees

3.1 EMSL Management

As shown in Figure 3.1, EMSL management is comprised of a Director, two Associate Directors, and an EMSL Operations Manager. In addition, 11 Technical Leads are responsible for the capabilities, staff, and user program within their assigned groups. Finally, two advisory committees, the Science Advisory Committee and the User Advisory Committee, provide guidance and expertise to EMSL management.

Specific roles, responsibilities, accountabilities, and authorities for all components of EMSL management are outlined in detail in Appendix A.

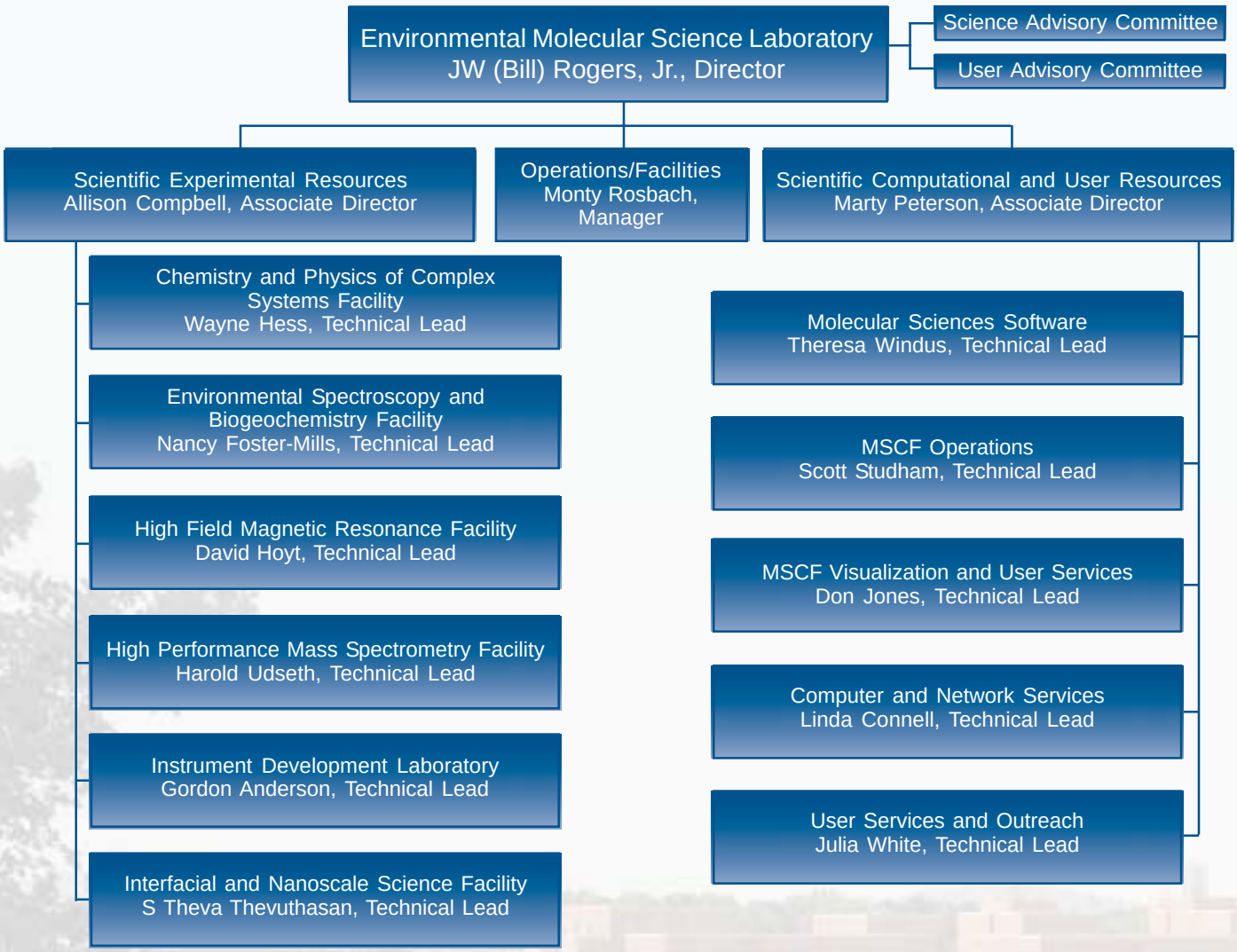


Figure 3.1. EMSL organizational structure

3.1.1 EMSL Director

The primary role of the EMSL Director is to oversee the activities of the Associate Directors and to work with external committees to design and implement EMSL's strategic plan and vision. The EMSL Director is ultimately responsible for all aspects of EMSL's environment, safety, and health program (ES&H) as well as stewardship of the user program.

3.1.2 EMSL Associate Directors

EMSL is assigned two Associate Directors: one for Scientific Experimental Resources, and another for Scientific Computational and User Resources. These Associate Directors provide direct oversight of EMSL facilities and staff, and are responsible for implementing EMSL's strategy and user program.

3.1.3 EMSL Operations Manager

The roles, responsibilities, accountabilities, and authorities of the EMSL Operations Manager are discussed in detail in Appendix A.

3.1.4 EMSL Technical Leads

The roles, responsibilities, accountabilities, and authorities of the EMSL Technical Leads are discussed in detail in Appendix A.

3.2 EMSL Advisory Committees

The Science Advisory Committee and User Advisory Committee are independent bodies charged with providing objective, timely advice to EMSL leadership. Both committees report to the EMSL Director.

3.2.1 Science Advisory Committee

The Science Advisory Committee is responsible for the following activities:

- Performing periodic reviews of the scientific impact of the elements of EMSL's user program. These elements include Collaborative Access Teams, Scientific Grand Challenges, requests for proposals, and unsolicited proposals (open access).
- Providing advice on long-range plans, priorities, and strategies to more effectively address the scientific aspects of EMSL's user program. This includes balancing allocation time among the elements of the user program (e.g., Collaborative Access Teams, Scientific Grand Challenges) and identifying potential new capabilities or scientific areas of research.
- Providing advice on the appropriate levels of funding and time allocation to develop the aforementioned plans, priorities, and strategies and to help maintain the appropriate balance among competing elements of EMSL.
- Providing advice to EMSL leadership on a variety of scientific and technical aspects, as requested by the EMSL Director. The Scientific Advisory Committee may seek outside input from or expand to include *ad hoc* members who can provide specific expertise about technical areas under discussion.
- Serving as DOE client advocates.

The nature of the goals and purposes of the Science Advisory Committee require it to be ongoing and dynamic. The committee meets a minimum of once per year, with membership of approximately 20 individuals appointed by the EMSL Director.

Subcommittees of the Science Advisory Committee may be formed to provide recommendations with respect to particular matters related to committee responsibilities. *Ad hoc* members external to the Science Advisory Committee may be appointed to ensure the competency necessary to conduct the subcommittee's business.

3.2.2 User Advisory Committee

The User Advisory Committee is responsible for the following activities:

- Providing advice on how to facilitate the effective use of EMSL. This includes advocacy for user interests as well as recommendations for integrating the various demands on EMSL equipment and staff resources to optimize use and impact.
- Providing advice on priorities and strategies to effectively address the multiple missions of EMSL. This includes exploring new paradigms for instrument use and user activity associated with EMSL's broad-based and often unique instrumentation resources.
- Advocating and promoting effective communication between EMSL leadership and the user community to help facilitate mutual understanding in support of achieving maximum impact by EMSL users.

The User Advisory Committee is comprised of twelve members and includes at least one experienced user in each of the six major research facilities of EMSL (see Section 4.0 for detailed information on each facility). Nominations for committee membership are solicited from EMSL's Technical Leads and Associate Directors. The User Advisory Committee is responsible for recommending to the EMSL Director the appointment of potential new members, and the EMSL Director is responsible for appointing committee members and selecting the committee chair. In general, committee appointments are made for a term of three years, with the potential for re-appointment to one additional term. *Ad hoc* subcommittees of the User Advisory Committee may be established to focus on specific areas requiring concentrated effort.

In order to secure continuity in committee activity, appointments are staggered so that one-third of the appointments is made at the beginning of each calendar year.

The User Advisory Committee meets two times a year at approximately six-month intervals. Every effort is made to schedule one of these meetings in conjunction with the annual Users' Meeting at EMSL to encourage direct contact between the committee and the broader user community. Additional meetings of the committee or any subcommittees are scheduled as needed to provide timely advice in support of optimizing EMSL's effectiveness.

The EMSL operations budget funds both advisory committees and is provided by the EMSL Director.

4.0 EMSL Facilities and Supporting Capabilities

EMSL is divided into six research facilities that are available, either individually or in combination, for user research. Additionally, EMSL houses an Instrument Development Laboratory, along with Computer and Network Services and User Services and Outreach groups. Each facility is equipped with state-of-the-art instrumentation and houses highly skilled staff who work in an interdisciplinary manner to support user research activities.

4.1 Experimental Resources

4.1.1 Chemistry and Physics of Complex Systems Facility

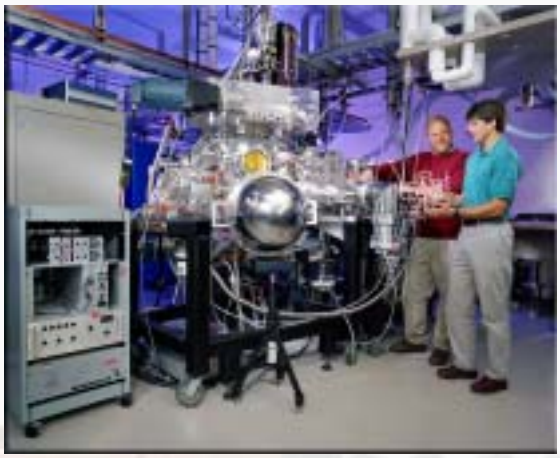
The Chemistry and Physics of Complex Systems Facility fosters fundamental research in the natural sciences to provide the basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use and contaminant releases.

Representative Research Activities

Researchers within this facility develop molecular information about processes occurring at the interface among environmentally important liquids, solids, and gases. In addition, they work to obtain a mechanistic understanding of chemical transformations of molecules and materials driven by thermal, radioactive, or optical sources. Additional themes of research within this facility include providing a molecular-level understanding of solvation and subsequent reactions in simple and complex systems related to the chemistry of complex wastes, contaminated solids and groundwater, and other natural systems; single-molecule spectroscopy and high-resolution imaging techniques for studying biological systems; and development of instrumentation for real-time analyses of chemical and biological natural or human-made species.

Research Capabilities

- Molecular beam surface dynamics and kinetics
- Ion soft landing interfacial transport
- Electron and photon excited non-thermal interfacial chemistry systems
- Single-molecule and non-linear imaging microscopy systems
- Systems for molecular-scale synthesis and characterization of model materials
- Electron microbeam for live-cell radiation biology research
- Environmental scanning electron microscope.



4.1.2 Environmental Spectroscopy and Biogeochemistry Facility

The Environmental Spectroscopy and Biogeochemistry Facility is involved in experimental and modeling studies of chemical phenomena and mechanisms on mineral and microbe surfaces and on complex heterogeneous environmental materials from soils, sediments, and groundwater zones.

Representative Research Activities

The research performed in this facility results in improved microscopic models of environmental processes that can be applied to the real world. Research capabilities include materials characterization, aqueous-phase and solid-phase speciation and reaction/kinetic measurements, analytical environmental chemistry, modeling of molecular and thermodynamic geochemical processes, and large-scale reactive-transport studies. A research staff with broad interests in mineral surface chemistry, biogeochemistry, thermodynamics, environmental spectroscopy, and molecular modeling are housed in the facility and are available for collaborative research and to assist users in integrating results of experiments and modeling.

Research Capabilities

- Laser-induced fluorescence, nonlinear, photoacoustic, Raman, and ultraviolet-visible spectrometers, streak camera, confocal microscope, and lasers
- Near-mid-far Fourier transform infrared spectrometer/microscope
- Mössbauer and electron paramagnetic resonance (EPR) spectrometers
- Scanning tunneling and atomic force microscopes
- Multifluid flow/transport cells
- Geochemistry molecular modeling software
- General analytical equipment.

4.1.3 High-Field Magnetic Resonance Facility

The High-Field Magnetic Resonance Facility is equipped with state-of-the-art nuclear magnetic resonance (NMR) and EPR instrumentation for determining molecular structures that impact environmental remediation and biological health effects.

Representative Research Activities

Staff within this facility offer expertise in the areas of structural biology, solid-state materials/catalyst characterization, magnetic resonance imaging techniques, and high-resolution spectroscopy of biological objects using slow (1 to 100 Hz) magic angle spinning. Research activities include structure determination of large molecular assemblies such as protein, DNA (normal and damaged), and RNA complexes as a cellular response to chemical or radiological insults; conformational changes in membrane protein complexes involving metal clusters as followed by pulsed EPR; NMR-based structural and functional genomics; materials and catalyst characterization via solid-state techniques; non-invasive biological imaging, integrated magnetic resonance and confocal microscopy; and slow spinning NMR to study cell systems.

Research Capabilities

- Twelve NMR spectrometers (ranging from 300 to 900 MHz) and one pulsed EPR spectrometer, with capabilities in high-field liquid-state, solid-state, and micro-imaging techniques

- Combined optical and magnetic resonance microscope
- Low-temperature probes for metallo-protein chemistry and structure
- Virtual NMR capability to allow remote users to use and collaborate over the Internet with EMSL scientists via Secure Shell.

4.1.4 High-Performance Mass Spectrometry Facility

The High-Performance Mass Spectrometry Facility provides cutting-edge mass spectrometry capabilities that focus on global proteomics research and allow visualization and analyses of proteins of a cell in greater detail than before.

Representative Research Activities

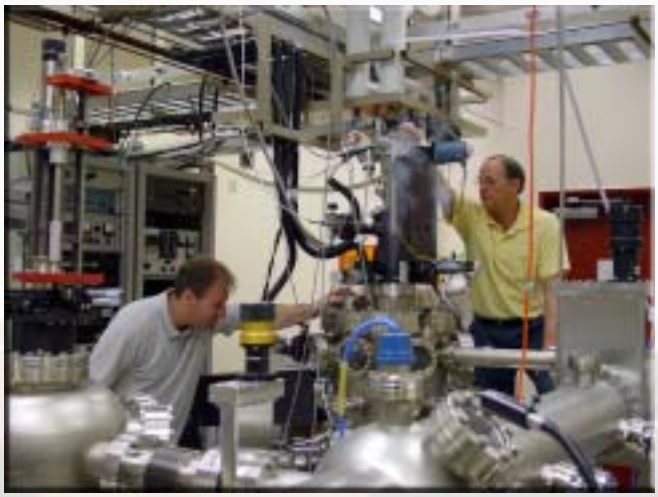
This facility provides state-of-the-art instrumentation for challenging research in areas such as proteomics, cell signaling, cellular molecular machines, and high-molecular weight systems, in general. The research activities conducted within this facility include proteomic analyses of whole cell lysates, analyses of organic macromolecules and protein complexes, quantitation using isotopically labeled growth media, targeted proteomics analyses of subcellular fractions, and nucleic acid analysis of RNA and DNA oligomers. The facility's capabilities of providing very-high-sensitivity and high-resolution mass spectrometry and very-high-resolution separations greatly benefit these areas of research and are enhanced by the capabilities listed below.

Research Capabilities

- Four Fourier transform ion cyclotron resonance mass spectrometers, 3.5, 7, 9.4, and 11.5 Tesla with electrospray ionization sources
- Sciex QSTARR quadrupole time-of-flight mass spectrometer
- Five Finnigan LCQ ion trap spectrometers
- Finnigan TSQ 7000 triple quadrupole spectrometer
- Ultrahigh-pressure liquid chromatographs.

4.1.5 Interfacial and Nanoscale Science Facility

Staff in the Interfacial and Nanoscale Science Facility research a variety of oxide mineral films and interfaces, nanoscale materials, and electronic and catalysis materials. Capabilities within this facility are used to conduct microfabrication and microanalytical separations and sensing.



Representative Research Activities

A unique environment is provided in this facility for research in areas such as nanoscience and nanotechnology; heterogeneous catalysis; environmental interfaces, including aerosols and minerals; materials interfaces and chemoselective interfaces; and areas within microanalytical science, such as chemical sensing and microfluidics. Portable deposition, electrochemical, and optical experimental stations located in this facility can be linked to analysis chambers to create unique experimental arrangements. Facilities are also available

for materials synthesis using thin-film deposition and chemical synthesis, ion beam processing and analysis, surface and bulk characterization, catalytic reaction, microfabrication, electron microscopy and X-ray analysis, and microanalytical systems development and testing.

Research Capabilities

- Molecular beam epitaxy and chemical vapor and sputter deposition
- State-of-the-art surface science tools
- High-resolution electron microscopes and X-ray diffraction instrumentation
- Ultrahigh vacuum, liquid, and ambient environment scanning probes
- Gas chromatography, NO_x analyzer, and RX100 testing and characterization system
- Research tools for microfabrication and clean room capabilities.

4.1.6 Molecular Science Computing Facility

The Molecular Science Computing Facility provides scalable high-performance computational resources for basic and applied research projects in environmental molecular science that address the environmental problems and research needs facing DOE and the nation.

Representative Research Activities

This facility provides computational resources for researchers at hundreds of sites across the world and allows use of object-oriented, massively parallel, and extremely scalable software developed by PNNL to conduct research and develop applications such as groundwater flow simulations; climate models; geochemical applications; modeling of chemistry on porous sites; heavy element chemistry; molecular thermodynamics and kinetics; prediction of excited states; nanotechnology; catalysis; biological membranes; and bioinformatics. A Graphics and Visualization Laboratory within the facility provides researchers with visualization capabilities of large data sets generated by the facility's state-of-the-art computing equipment.

Research Capabilities

- 1976 Itanium-2 processors with Quadrics Elan-4 interconnect (11.8 teraflops), 6.9 terabytes of memory, 450 terabytes of local disk, and 53 terabytes of global disk
- Molecular Science Software Suite, including Extensible Computational Chemistry Environment (a problem-solving environment for chemistry); NWChem (a massively parallel computational chemistry software package); and ParSoft (libraries and tools for interprocessor communications, high-performance input/output, and programming models for hierarchical memory systems)
- A SGI 3400 8 processor, graphics and visualization server with integrated video and audio editing system.

4.2 Computing and User Resources

4.2.1 Instrument Development Laboratory

Staff at the Instrument Development Laboratory design, develop, and deploy advanced state-of-the-art instruments and custom application software in support of ongoing research efforts at EMSL.

Representative Research Activities

Staff within this laboratory maintain a pool of laboratory testing and measurement equipment, data acquisition cards, software development tools, workbench space, and instrument fabrication tools for use by EMSL users. They provide user support from initial design through fabrication, testing, and deployment.

These staff have expertise in electronic circuit design and fabrication, and analog, high-speed digital, and radio frequency technologies. They work with researchers to provide key components and circuits that are unique or not otherwise available. Circuit design and analysis activities make use of, but are not limited to, MicroSim, PSpice A/D, Schematics, PC Boards, and PLSyn tools. Instruments are assembled and modified with hand and sheet-metal working tools in the prototype machine shop.

Instrument Development Laboratory staff also provide support in real-time data acquisition and instrument control, as well as data visualization and management. They have experience in a variety of programming languages, including Visual Basic, Java, C, C++, LabView, Assembly, Access, and SQL Server. In addition, software staff are familiar with a number of instrument control strategies, including GPIB, Serial (RS-232), IR, TCP/IP, Analog and Digital I/O, and high-speed event counting and timing.

Research Capabilities

- Electronics shop, workstations, tools, and user/staff assistance
- Parts and supplies, electronic components, and small hardware
- Test equipment checkout
- Custom software design, development, and support
- Data acquisition, instrument control, laboratory automation, and systems integration
- Data analysis and visualization, data management, and archiving
- Data management and automated data analysis
- Handheld and embedded systems
- Software modifications and bug fixes
- Research instrumentation fabrication and modification
- Electronics hardware design
- Control and monitoring software development
- Systems engineering
- Embedded control.

4.2.2 Computing and Network Services

The Computing and Network Services group is responsible for the operation and maintenance of EMSL's computing infrastructure, which provides an advanced computing environment that enables staff, visitors, and collaborators to effectively use computer and network resources to address research and business requirements. This group supports EMSL's growing business and research needs that pertain to information sciences and secure global information access.

Representative Activities

Staff within the Computing and Network Services group are responsible for a variety of tasks related to EMSL's computing infrastructure, including the following:

- Identifying, testing, benchmarking, and implementing emerging computing technologies
- Supporting office configurations for Windows and Macintosh systems
- Supporting Unix configurations for Sun, SGI, Linux, IBM, and Hewlett Packard systems
- Supporting email, calendaring, and printing
- Providing backup and restore services
- Providing auditorium, conference room, and multimedia audio-visual services
- Supporting computer equipment allocation and tracking
- Providing an email-based help system
- Providing web services
- Developing computing policies, security plans, and computer vendor contracts
- Managing scientific user accounts and access control
- Providing secure remote access from the Internet
- Providing scientific computing consultation and services
- Administrating Windows and Unix network infrastructure
- Supporting distributed file services and data management
- Designing and implementing distributed service applications
- Providing file and source code version control services
- Providing database services
- Supporting personal digital assistants and wireless devices.

Capabilities

- Design, install, configure, and maintain Windows, Macintosh, Unix/Linux hardware and software
- Conduct office, laboratory, workgroup, and clustered configurations
- Maintain network system architectures
- Develop security and remote access methodologies
- Develop distributed file systems
- Develop audio-visual hardware and software.

4.2.3 User Services and Outreach

The EMSL User Services and Outreach group provides support services to facilitate and promote the effective use of EMSL resources by staff and users. This group also plans, develops, and coordinates implementation of EMSL's communication strategy to promote the awareness, reputation, and use of EMSL as a national user facility.

Representative Activities

To achieve effective use of EMSL resources by staff and users, the User Services and Outreach group:

- Produces the EMSL annual and monthly reports
- Provides an overview and training for the EMSL User System
- Provides access control to the facility
- Distributes proximity cards and computer passwords to staff and users
- Schedules conference rooms for seminars, meetings, etc.
- Creates print media, such as brochures, newsletters, posters, fliers, and photos, that advertise EMSL's achievements and capabilities
- Creates and maintains electronic media and facility web sites
- Organizes the EMSL User Meeting and workshops
- Provides tours of EMSL.

5.0 Accessing EMSL

EMSL facilities and capabilities are available to the general scientific and engineering communities to conduct research in the environmental molecular sciences and other significant areas. Recognizing the wide variety of research needs, EMSL strives to provide a variety of seamless mechanisms for users to access its capabilities to solve problems that range from small, single private investigator projects to large, complex, multi-investigator scientific challenges.

EMSL supports both open and proprietary research:

- **Open research** is basic and applied research in science and engineering where the resulting information is ordinarily published and shared broadly within the scientific community. Users engaged in open research generally are not charged for using EMSL facilities or equipment. Intellectual property developed in the course of open research is protected in accordance with DOE policies, which, in general, assign the intellectual property and any resulting commercial benefits to the discoverer.
- A limited amount of **proprietary research** may also be conducted at EMSL under a proprietary sales contract. Under the terms of the DOE class waiver, users engaged in proprietary research are obligated to pay the full-cost recovery rate for use of the facility. In return, the user has the option to take title to any inventions made during the proprietary research program and to treat as proprietary all technical data generated during research.

Users may access EMSL facilities via several mechanisms, including Scientific Grand Challenges, Collaborative Access Teams, requests for proposals, and unsolicited proposals (open access). These types of access are discussed in detail below. All users must sign an EMSL User Agreement and agree to abide by the terms of the User Agreement prior to using EMSL facilities or capabilities. All users must also be cognizant of, and abide by, EMSL standard practices and procedures.

General support and appropriate training of the facilities or capabilities required will be provided to users by EMSL staff. Scheduling of these resources is determined by EMSL staff in consultation with the users.

5.1 Scientific Grand Challenges

Beginning in Fiscal Year 2004, EMSL is implementing two or more Scientific Grand Challenges—an effort to answer important scientific questions through a collaborative approach, using EMSL capabilities. These Scientific Grand Challenges are expected to increase the scientific impact and robustness of EMSL as a user facility and PNNL's scientific programs. They will be consistent with DOE mission areas; will be focused on critical milestones in the advancement or use of science; will be user driven; and will take full advantage of the unique capabilities, resources, and technical expertise available at EMSL to address significant problems. The scope of the scientific problems to be addressed will require multidisciplinary teaming, and their breadth will be of such magnitude that they cannot be addressed at any other existing single facility. The challenges will require not only the capabilities of EMSL, but possibly other DOE user facilities and specialized instrumentation and capabilities at the participants' home institutions. They will require significant

management and coordination to meet their aggressive goals, and are expected to attract and involve users who are among the best scientists in the world. The Scientific Grand Challenges will generally have a set of well-defined goals in capability development or scientific impact and will have a specified duration.

5.1.1 Implementation

The Scientific Grand Challenge themes will be determined by the scientific community through EMSL's Science Advisory Committee together with selected external experts in the theme area. The EMSL Director and Associate Directors, along with PNNL scientific staff, will coordinate development of these theme areas and submit them for approval to the appropriate DOE program offices. The process for implementing a Scientific Grand Challenge will involve the following:

- A steering group for each theme will be established that is comprised of external experts in the theme field and EMSL/PNNL staff.
- The steering group will work closely with the appropriate DOE program offices to develop preliminary Scientific Grand Challenge themes and then organize one or more workshops centered around these themes. The workshops—to be held at EMSL—will broadly represent the appropriate scientific field and will be facilitated to efficiently converge on candidate Scientific Grand Challenge themes. They will be designed to highlight EMSL capabilities to those who are not familiar with them and to provide insight into use of these capabilities.
- A written document will be prepared summarizing the content of the workshop and condensing and focusing the outcome from the workshop into one or more Scientific Grand Challenge themes. Subsequent activities include developing strategic plans and roadmaps for each executed challenge.

5.1.2 Schedule

The schedule for organizing and implementing EMSL's first two Scientific Grand Challenges has been ongoing as follows:

Activity	Fiscal Year/Quarter
Establish Science Advisory Committee	Fiscal Year 2003, Second Quarter
Establish Steering Groups	Fiscal Year 2003, Third Quarter
Host Workshops	Fiscal Year 2003, Third Quarter
Workshop Report to DOE Program Offices	Fiscal Year 2003, Third and Fourth Quarters
Call For Proposals from DOE Program Offices	Fiscal Year 2003, Fourth Quarter
Begin Scientific Grand Challenges	Fiscal Year 2004, First Quarter

5.1.3 Funding

The funding necessary to support the Scientific Grand Challenges will be provided by EMSL, the existing research funds of participants, and the DOE program offices as necessary to supplement existing research funds.

5.2 Collaborative Access Teams

Collaborative Access Teams (CATs)—comprised of teams of scientists nationwide—are formed to conduct high-impact scientific research in a focused theme that demonstrates the capabilities and value of EMSL and maintains EMSL at the forefront of science. CATs provide a mechanism to attract and increase the number of high-impact users in a focused research environment and build new capabilities for use by the team and general users.

Membership in a CAT is open to all individuals within the scientific community who can contribute significantly (e.g., funding, equipment, design and engineering, operations manpower, etc.) to the CAT. Individual scientists interested in becoming a member of a CAT must contact the CAT lead.

The CAT lead is responsible for submitting a CAT proposal and acting as the contact for all CAT activities. Additionally, the CAT lead has the responsibility to:

- Determine membership
- Provide and build advocacy of EMSL science and capabilities
- Build user communities around the CAT
- Attract leading scientists as users to enable high-impact science
- Integrate EMSL scientists in programmatic research, as appropriate
- Encourage the broad use of EMSL capabilities
- Report and track progress and results.

In return, CATs will receive:

- Guaranteed use of EMSL facilities, as advised by the Science Advisory Committee
- The ability to compete for additional time using EMSL's proposal process
- EMSL funding to build and market the CAT to the external user communities, as determined by the EMSL Director and Associate Directors
- High priority for space within EMSL
- The option to request EMSL funds for capability development. This effort will be coordinated and managed through the appropriate Technical Lead.

CAT calls for proposals and resulting teams will be announced to the scientific community in a variety of ways, including through the EMSL external website, by email to EMSL users and the various scientific societies, and by posters located at scientific society meetings.

5.2.1 Implementation

CAT leads are required to submit a CAT proposal to the EMSL Director's Office for consideration. Proposals should be sufficient in detail and describe the following components:

- CAT lead and members (including external researchers and EMSL/PNNL staff)
- A description of the research

- The expected outcomes and impacts (e.g., publications—including percentage of publications with outside collaborators; high-visibility users and collaborators; intellectual property; and education)
- A description of new capability development activities. This information must identify the EMSL facility where the capability will be housed and the associated Technical Lead.
- A list of required EMSL capabilities and instruments and the time requested for use
- A description of research programs that support the CAT, to include the title of the funding source; budget (e.g., $2M labor, $0.3M in expenses); staffing (e.g., six full-time equivalents and six full-time equivalent postdoctoral fellows); and capital investment
- Budget requests to EMSL, including CAT lead funding (e.g., travel, time) and capability development.

CAT proposals will first be reviewed by the EMSL Director and Associate Directors, and then by the Science Advisory Committee for scientific merit, appropriateness of the proposed method or approach, relevance to the problems and research needs of DOE and the nation, appropriateness of proposed resources, and the technical competence of the investigators. The Technical Leads, User Advisory Committee, and/or Science Advisory Committee will also provide advice on the allocation of time to the requested resources, and will formally review all CATs every three years. In addition, a progress report will be submitted annually to the EMSL Director, who can formally review the CAT at a subsequent User Advisory Committee and/or Science Advisory Committee meeting if it is determined that the CAT is not meeting expectations.

5.2.2 Schedule

To organize and implement CATs, proposals will be due at the beginning of each fiscal year, with review and implementation occurring during the first quarter of the fiscal year.

5.2.3 Funding

A small amount (~$35K) of EMSL funding will be provided to the CAT lead for time and travel expenses as a result of attracting users to the CAT. EMSL funding may also be allocated for capabilities development within the CAT (as determined by the Science Advisory Committee). These funds will be managed through the appropriate EMSL Technical Lead. CAT team members' time and supplies will be funded through the CAT programmatic resources and not through EMSL. The host CAT will provide each external user with programmatic funding to receive the technical training and support required to use the instrumentation to which the user has been granted access, unless prior commitments have been made by the Technical Lead.

5.3 Requests for Proposals

Currently, EMSL's High-Field Magnetic Resonance Facility and Molecular Science Computing Facility generate regular requests for proposals.

5.3.1 High-Field Magnetic Resonance Facility

The High-Field Magnetic Resonance Facility (http://www.emsl.pnl.gov/hfmrf/) generates two requests for proposals per year, due on January 15 and July 16. The preferred method of submission is electronically using EMSL's proposal form.

To enable an effective and complete proposal review, potential users of the High-Field Magnetic Resonance Facility are asked to provide the following information in their proposals:

- Significance of the proposed work
- A summary of progress to date, with an indication as to why EMSL resources are essential for completing the proposed research
- Justification of the length of time requested
- A list of needed experiments
- A description of any novel requirements to perform the experiments or handle samples
- Delineation of any need for chemistry/biochemistry preparation labs to facilitate sample preparation
- Any safety requirements or risks associated with sample handling, storage, or preparation.

Proposals are first reviewed by EMSL staff for appropriateness and then forwarded to an external panel for review. Review and acceptance is based on the quality of the proposed science, the appropriateness of the requested instrumentation, and the contribution of EMSL in bringing that science to fruition. If the proposal is granted, EMSL staff will assign a time allocation, and the user will be notified.

5.3.2 Molecular Science Computing Facility

Proposals for using computing resources at the Molecular Science Computing Facility (http://www.mscf.emsl.pnl.gov/) are categorized as either Pilot Projects or Computational Grand Challenge Projects:

- **Pilot Projects** are proposals of general research (non-Computational Grand Challenge) requiring a maximum of 75,000 processor hours, with a maximum duration of one year. On average, Pilot Projects are allocated 33,000 processor hours. These projects are typically focused on developing the capability to submit a Computational Grand Challenge proposal in the future (e.g., a combination of theory/method or code development activities or calculations that provide the initial scientific basis of a Computational Grand Challenge proposal). Allocations for Pilot Projects are at times limited, depending upon existing commitments. Prospective authors of Pilot Projects should first contact the facility to gauge availability of requested resources. Proposals that are received where resources are not available will be held until resources do become available.
- **Computational Grand Challenge Projects** focus on examining complex problems in science and engineering with broad scientific and environmental or economic impacts, and the solutions to these problems can be advanced by applying high-performance computing techniques and resources. Only a few large proposals are accepted each year. The duration of Computational Grand

Challenge Projects range from one to three years. Proposals to the Molecular Science Computing Facility are open to all researchers, independent of funding sponsors. These projects are comprised of multiple investigators from universities, national laboratories, other government laboratories, and industry working in collaboration.

Review and acceptance of Computational Grand Challenges and Pilot Projects are based on scientific merit, appropriateness of the proposed method or approach, relevance to environmental problems and research needs of DOE and the nation, technical competence of the investigators, and reasonableness and appropriateness of use of proposed computer resources. Investigators must address these criteria in their proposals.

5.4 Open Access

Potential users may at any time submit a proposal for use electronically through the EMSL website (http://www.emsl.pnl.gov). All proposals are reviewed and accepted based on scientific merit, appropriateness of the requested facility, relevance to DOE's missions, and credentials of the principal investigator. Following submission, the proposal author will receive a prompt receipt of acknowledgment and, in most cases, will be advised within four weeks whether the proposal has been accepted. Appeals, questions, and proposal review comments may be addressed in writing to the EMSL User Services Office (mailto:userservices@emsl.pnl.gov). Authors will receive a timely written response. If the proposed use is approved, the EMSL host will contact the user to coordinate arrangements. Users are requested to advise their hosts of any materials, chemicals, or equipment to be shipped or hand delivered to EMSL.

6.0 Operating System

The increase in the number of EMSL users results in an overall impact to user services and facility operations. EMSL facilities are in increased demand; proposal processing and tracking becomes more complex; integrating the various training and access requirements becomes increasingly problematic; and tracking scientific accomplishments of a diverse, growing user community becomes more difficult. To improve user services, the following critical outcomes must be achieved:

- An environment must continue to be created that enables EMSL users to access and use the facility with minimal delays. Thus, user services such as training, computer access, and badging must be performed timely and seamlessly.
- Systems that capture and track user proposals, facility use, user satisfaction, user contact information, and user publications must be upgraded and enhanced.

6.1 Integrated Operations System

To achieve the goal of seamless and timely services, EMSL developed the Integrated Operations System (IOPS), a web-based software tool that helps facility users throughout PNNL effectively implement building-specific ES&H programs.

The IOPS approach is to create an operational environment that is enabling for the research staff and mission. Key staff are given responsibility, authority, and the tools to take the necessary actions for making work proceed efficiently and flexibly with a reduced need for oversight within defined boundaries. Research staff work with PNNL's Facilities and Operations and Environment, Safety, Health and Quality staff to ensure that *safe work practices* for a facility are rooted in performance rather than rote ES&H compliance.

Implicit in this approach is the conviction that compliance with regulations, while important, is not sufficient to ensure safety. Rather, safety results from the acceptance of responsibility and accountability by individual staff members who integrate safe work practices into their daily operations.

All users of facilities that implement IOPS are responsible for knowing and implementing the safety requirements applicable to their own work. However, the responsibility for managing work safely in a workspace is clearly assigned to one person: the cognizant space manager. As the workspace owner/user who has the most investment in day-to-day operations, the cognizant space manager is at the most effective level to make day-to-day decisions about workspace use. They are responsible and accountable for evaluating workspace hazards, determining work practices needed to control those hazards, and ensuring that workspace users have sufficient hazard awareness training before they work unescorted in the workspace.

To assist cognizant space managers with evaluation of potential hazards, IOPS creates a Hazard Awareness Summary that allows them to describe the hazards and associated controls. In addition, to evaluate the applicability of the ES&H program in a workspace, the cognizant space manager or their delegate periodically conducts a self assessment by using an IOPS-generated Self-Assessment Checklist.

Cognizant space managers are authorized to make decisions regarding their workspaces. Thus, they can approve or disapprove workspace activities, approve or revoke a workspace user's access to the workspace, and correct ES&H deficiencies in the workspace.

Finally, to facilitate seamless and timely services, IOPS is equipped with a user registration process so that PNNL staff can host facility users, and allows for the ability to request a security badge and computing services as needed. Hosts and other PNNL staff can also request unescorted access to a workspace for themselves or for the individuals they host, with the cognizant space managers providing final authority to grant or deny access to the workspaces under their control. They also specify each user's training requirements based on the types of interactions each will encounter with hazards in the workspace.

6.2 EMSL User System

The EMSL User System was designed to provide users with a method for requesting access to EMSL capabilities and facilities, and to provide management with an effective way to track users, project uses, and results. Potential users must read and agree to the terms and conditions for using EMSL before proceeding with an electronic proposal request via the EMSL external website.

In the proposal system, the potential user is asked to provide information to three web pages: the Participants, Details, and Logistics pages.

- The **Participants** page requests information about each participant and their related institutions. It allows all participants to be included and for the designation of one participant as the Primary Author.
- The **Details** page requests the proposal title, abstract, proposed start and end dates, facility requested, and EMSL resources along with their estimated hours of use.
- The **Logistics** page requests information about the funding agencies, samples, chemicals, and user equipment that will be brought to the facility. It also provides a space for comments.

Figure 6.1 depicts the proposal lifecycle. The proposal process begins when a proposal is received by EMSL and ends when the proposal is either approved and the start date is reached, or when it is denied or withdrawn. This process typically takes days to complete. The status of a proposal in this stage is submitted, pre-approved, or approved:

- **Submitted**: The proposal has been entered into the EMSL User System, but a host has not yet been assigned.
- **Pre-approved**: A host has been assigned, but not all approvals have been received.
- **Approved**: All approvals have been received, but the start date has not yet been reached.

Once approved, staff within the applicable facility schedule use. When in the "Usage Stage," the proposal is considered active. Accurate start dates must be provided to the EMSL User System, as this information is reported quarterly to DOE. Start dates cannot be adjusted in the EMSL User System if the proposal has been active for a year or longer. Proposals that are active for more than one year must be extended annually by the host. The primary author will also receive an annual email requesting a year-end summary.

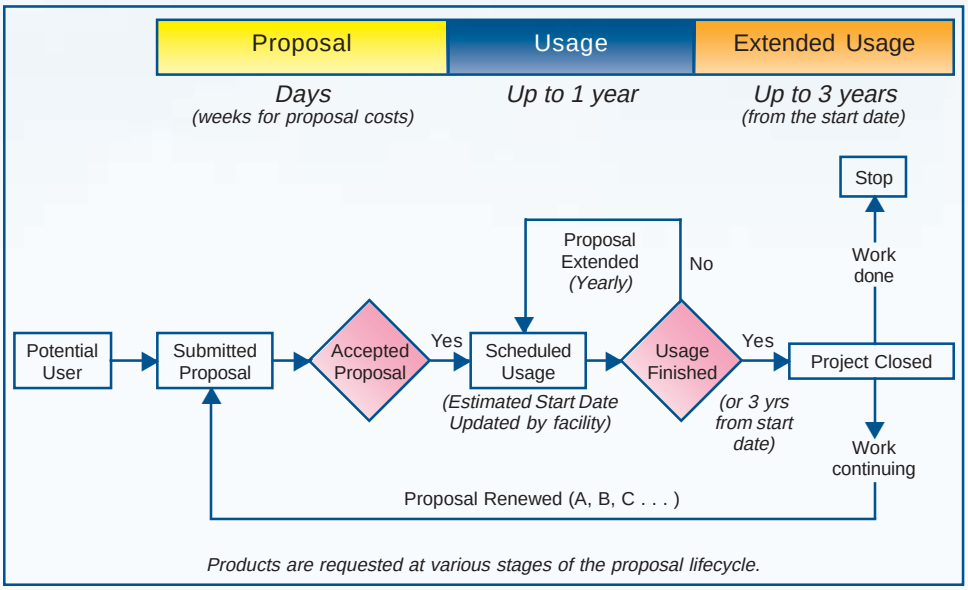


Figure 6.1. EMSL Proposal Lifecycle

A proposal can only be maintained in the Usage Stage for three years, when it will automatically be closed. However, an EMSL user or staff member acting as their delegate can reload the proposal and request to renew it, whereupon it will once again undergo the required review/approval process.

A proposal is reviewed and can be denied by any of the following five approval bodies:

- The EMSL Business Office reviews proposals to determine whether the user agrees to the terms of EMSL's Non-Proprietary User Agreement and its Appendix B.
- Staff from the applicable EMSL facility review proposals to determine whether the proposed research has scientific merit and is appropriate for the requested instrumentation.
- The EMSL Safety and Health Representative reviews proposals for potential hazards related to materials (e.g., chemical hazards) to be brought onsite by the potential user.
- Environment, Safety, Health and Quality staff review proposals to determine whether the proposed research will have potential environmental impacts.
- The Human Subject Review Board reviews proposals to make certain that human subjects policies (e.g., does the proposed research involve human tissue or other human sample types) are followed as appropriate.

Proposals can be withdrawn by any EMSL staff member.

Even if an estimated end date has passed, the proposal is not marked as closed until the host or their delegate closes it in the EMSL User System (or the three-year period has been reached).

6.3 EMSL Resource System

The EMSL Resource System (Figure 6.2) is a web-based tool that tracks the use of EMSL's major instruments and facilities. Design and development of the EMSL Resource System began in early Fiscal Year 2002, with all facilities tracking major instrument use beginning in 2003. An algorithm for defining use of the large variety of instruments tracked in the EMSL Resource System has been established, and the system has been enhanced to generate reports breaking down quarterly or annual use by usage type.

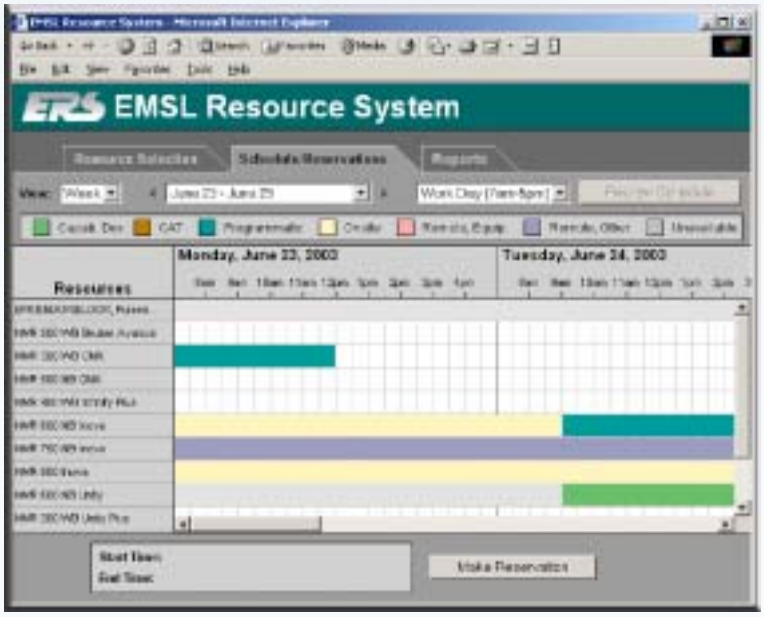


Figure 6.2. EMSL Resource System

6.4 ERICA

ERICA—Electronic Records and Information Capture Architecture—is an online tool that allows staff to search and retrieve records, scientific and technical information (e.g., publications, presentations), and intellectual property from their own workstations in minutes. The system:

- Automates and tracks PNNL's information release process from initiation through receipt of approvals and to the point of publication/public release. ERICA also assigns a clearance number to the product.
- Captures key information about publications/presentations by EMSL users.
- Captures key data about information released externally (to the public) by PNNL authors.
- Provides cleared information to other online systems that harvest and display scientific citations, such as ISI's Web of Knowledge and the Office of Scientific and Technical Information databases.
- Makes this information easily available to organizations within PNNL and to staff and managers who need to know the "bibliometrics" (e.g., research areas being represented by publications; who is authoring/releasing information; what information has been released by a given author, year, topic, or product type) for the Laboratory or who are producing contribution reports depicting what publications, awards, or intellectual property have been produced/released by a staff member, group, or project.
- Facilitates submitting and retrieving records from the desktop through the Total Records Information Management subsystem. This subsystem enables the capture, management, and control of documents from the point of creation through disposition. It provides an electronic repository for unclassified electronic records and document storage, change control for workflow processes, a retrieval tool for finding records/documents, and an archiving feature.

ERICA supports the strategies of two of our major clients, DOE and the Department of Defense, who are transitioning from paper-based, centralized repositories to cost-effective, distributed electronic access systems. Another client, the U.S. Nuclear Regulatory Commission, has also expressed interest in such electronic delivery mechanisms. ERICA will constitute PNNL's portion of DOE's national pointer system for the publicly available, electronic documents created at its national laboratories.

For further information regarding the policies and guidelines contained in ERICA, see http://erica/erica/default.asp.

7.0 Budget Allocation and Space

7.1 EMSL Budget Charging Guidelines

The complete formal document that addresses EMSL charging guidelines is contained in Appendix B and is summarized below.

EMSL's largest single source of funding is its operations budget. These funds are not a form of overhead, such as management or marketing funds; rather, they are fully burdened DOE programmatic funds. Just like hundreds of other PNNL programs, any charges to operations must support a programmatic mission. In this case, the mission is to support EMSL's role as a designated user facility.

To fulfill EMSL's mission, the operations budget funds a portion of EMSL staff time to perform work that contributes to users' research projects. Staff who charge to this budget must be performing work that meets the following funding intent:

- Procuring service contracts for EMSL scientific systems
- Maintaining EMSL scientific systems
- Managing EMSL laboratory space
- Training or assisting users on EMSL scientific systems, or operating systems for users
- Building new capabilities in support of EMSL
- User outreach
- Communicating and marketing EMSL's user program
- Supporting EMSL's user and resources tracking systems
- Managing EMSL's facilities
- Managing DOE's and EMSL's reporting requirements.

Funding from the operations budget cannot be used to cover the time of underfunded staff, if they are not performing work that meets the above criteria.

The future of EMSL's operations budget depends on the users the facility attracts and the resulting scientific impact of those users. Thus, EMSL management must make hard decisions regarding budget allocations. Preferred users conducting impactful science, as well as facilities, laboratories, and equipment that are highly used, will receive priority funding.

7.2 EMSL Space Use

EMSL space is overseen and managed by the EMSL Director and will be governed by the EMSL Space Occupancy Policy (Appendix C).

The EMSL Space Committee is comprised of the EMSL Operations Manager and appointed representatives from each of the research directorates in residence. Current committee members include Rich Barchet, Atmospheric Sciences; Carrie Ingersoll, Biological Sciences; Sue Finch, Chemical Sciences; Deb Gracio, Computational Sciences; Tobe Taylor, EMSL; and Monty Rosbach, EMSL Operations Manager.

Appendix A — Roles, Responsibilities, Accountabilities, and Authorities

Managers at the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) are assigned several roles, responsibilities, accountabilities, and authorities for the effective operation of the facility. In these instances, **role** outlines the function(s) that an individual plays in the organization. **Responsibilities** is defined as the obligation of the individual to ensure initiation, implementation, and completion of activities. **Accountabilities** means that the individual is answerable to a specific position or individual for fulfilling a responsibility for which they have authority to act. Finally, **authorities** outlines the decision-making powers and controls required by the individual to fulfill responsibilities without concurrence or approval of others.

EMSL Director

Role: Director of EMSL

Responsibilities:

- Manage the relationship with EMSL's U.S. Department of Energy steward
- Provide EMSL's Associate Directors with quality performance feedback and support long-term professional development or personal development goals
- Engage officials of universities nationwide to build a user program
- Attract and build a world-class scientific user base
- Oversee both EMSL advisory committees—the User Advisory Committee and Science Advisory Committee
- Set EMSL's scientific directions and develop EMSL's strategic plan
- Provide appropriate training and motivation to staff for gaining leadership and technical skills
- Communicate EMSL's strategies and goals to staff
- Create and maintain a supportive work environment
- Assess the performance of the EMSL organization, and take action to correct or improve performance, as necessary
- Approve procurements of larger than $1M
- Institutionalize EMSL's environment, culture, and resources to provide strong management and staff commitment to safe, secure, and environmentally compliant operations.

Accountabilities:

- To EMSL staff for creating and maintaining a safe and quality work environment
- To the EMSL Associate Directors for resource management and professional growth opportunities
- To the Level 1 Managers of the research directorates in residence for maintaining safe, effective, and compliant operations

- To the Pacific Northwest National Laboratory (PNNL) Director for stewardship of EMSL's user program.

Authorities:

- Approve allocations of EMSL's operations budget
- Take needed actions to provide safe, secure, and environmentally compliant operations
- Execute capability development strategies for staff, equipment, and facilities
- Approve staffing actions.

EMSL Associate Directors

Role: Associate Director of EMSL

Responsibilities:

- Oversee EMSL's user program
- Develop and allocate EMSL's operations budget for their areas of responsibilities
- Implement the actions outlined in EMSL's strategic plan
- Provide quality performance feedback to EMSL's Technical Leads and support long-term professional or personal development goals
- Provide appropriately trained and motivated staff to assist EMSL users
- Build and maintain a supportive work environment
- Provide the required resources for staff to maintain and be fully committed to safe, secure, and environmentally compliant operations
- Manage assigned resources (i.e., people, equipment, and facilities)
- Work with the EMSL Director to identify future resource needs.

Accountabilities:

- To assigned staff for quality of the work environment
- To assigned staff for resource management and professional growth opportunities
- To the EMSL Director for safe, effective, and compliant operations
- To the EMSL Director for stewardship of assigned technical resources and quality products and services.

Authorities:

- Authorize budget allocations (as delegated by the EMSL Director)
- Hire and assign EMSL Technical Leads
- Evaluate staff performance and take corrective actions, as needed
- Administer staff reward, incentive, and discipline systems consistent with PNNL policy

- Allocate assigned discretionary resources to achieve a capability development strategy
- Take action to mitigate hazards or safeguards and security threats/risks associated with work conducted by assigned staff
- Take action to provide safe, secure, and environmentally compliant operations.

EMSL Operations Manager

Role: Operations Manager of EMSL

Responsibilities:

- Provide a valued, staff-owned, intuitive, integrated, and self-managing environment, safety and health (ES&H) program
- Provide a working environment that includes adequate office, conference, research, and support facility resources to support EMSL programs
- Facilitate effective and cost-efficient support services within EMSL
- Manage assigned resources, such as people, equipment, and facilities
- Work with the EMSL Director and Associate Directors to identify future resource needs.

Accountabilities:

- To EMSL staff and management for the safety and quality of their work environment
- To EMSL staff and management for effective and cost-efficient support services
- To assigned staff for resource management and professional growth opportunities
- To EMSL staff and management for stewardship of assigned technical resources and quality products and services.

Authorities:

- Hire and assign staff to support EMSL operations. Identify and recommend individuals for EMSL cognizant space manager and facilities services positions
- Evaluate EMSL operations staff performance and take corrective actions, as needed
- Administer staff reward, incentive, and discipline systems consistent with PNNL policy
- Assign and reassign EMSL office and laboratory space to support EMSL missions
- Identify and fund, as appropriate, facility modifications that support EMSL missions
- Allocate assigned funds
- Take action to mitigate hazards or safeguards and security threats/risks associated with work conducted by assigned staff
- Take action to provide safe, secure, and environmentally compliant operations.

EMSL Technical Leads

Role: Technical Leads of EMSL's user facilities and support groups

Responsibilities:

- Enable the user program within the assigned facility or group
  - Develop and manage the user proposal review process
  - Assign appropriate staff to work with users, support operations, or enable outreach activities
  - Allocate and track the facility's instrumentation and staff time to users
  - Track user data and products
  - Ensure that data in the EMSL User System is accurate and current
  - Determine the needs of users and develop capabilities with respect to those needs
  - Properly use the allocated budget
  - Develop a strategic plan for the applicable facilities or groups as part of EMSL's overall strategic plan.
- Help staff find their role in the overall strategy and direction of the organization
  - Provide the opportunities and resources necessary for staff to be competent, trained, and qualified for assigned work
  - Effectively utilize, reward, and motivate staff
  - Evaluate staff performance and take corrective actions, as needed
  - Ensure that staff have available to them the appropriate professional growth opportunities (e.g., proposal development, scientific/technical meetings).
- Ensure safe and efficient operation of assigned resources
  - Develop an appropriate financial model for the assigned resources
  - Appoint cognizant space managers and provide resources to maintain safe and compliant workspaces
  - Determine that mitigation controls are in place for all identified hazards
  - Implement safeguards and security using approved work control processes, tools, and procedures.

Accountabilities:

- To assigned staff for the safety and quality of their work environment
- To assigned staff for resource management, capability development, and professional growth opportunities
- To the EMSL Associate Directors for stewardship of assigned resources and delivery of quality services
- To the EMSL Associate Directors for the appropriate implementation of safeguards and security measures.

Authorities:

- Assign staff to work with users, support operations, and enable outreach activities
- Evaluate staff and hold them accountable for performance; take action to correct or improve performance
- Allocate assigned funds
- Take action to mitigate hazards and/or safeguards and security threats/risks associated with work conducted by assigned staff.

Appendix B — Charging Guidance for EMSL User Facility Staff

This appendix provides staff of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) (organization code D7E2X) with information for determining when to charge to EMSL's operations budget and when to charge to projects that use EMSL resources.

EMSL's operations budget, comprised of U.S. Department of Energy programmatic funds, provides for the full operation and maintenance of EMSL as a user facility. The operations budget supports the following activities and items.

EMSL Operations Budget

EMSL Staff Labor

EMSL staff who work to maintain the facility and equipment in a ready-to-use, safe operating mode charge to the operations budget. Activities covered by this budget include the following:

- Assembling and disassembling equipment
- Configuring equipment
- Developing software
- Replacing, upgrading, and repairing (including emergency repair) equipment
- Performing routine maintenance of equipment
- Training users on equipment, instruments, and procedures
- Assisting users during experiments with instruments that require constant monitoring
- Assisting users with preparing their samples for analysis
- Evaluating and monitoring the progress of EMSL user proposals
- Managing laboratory space
- Assisting users with data analysis and interpretation
- Contributing to publications or reports
- Attending conferences, workshops, vendor shows, and seminars where knowledge is gathered related to maintaining or advancing EMSL capabilities or promoting EMSL.

Other Labor

Other labor, such as that provided by PNNL Crafts Resources staff and Fluor Daniel services, may be charged to the EMSL operations budget to support the activities listed above.

Non-Labor Items

The EMSL operations budget is also used for non-labor items needed to maintain EMSL and its equipment in a ready-to-use, safe operating mode. These charges include procurements, subcontracts, travel, service center requests, and other related costs, such as:

- Maintenance and services agreements assigned to EMSL equipment
- Consumables (e.g., liquid helium, nitrogen) required to keep equipment operating
- Laboratory and equipment supplies, such as latex gloves, test tubes, and slides
- Travel costs related to attending conferences, workshops, vendor shows, and seminars where knowledge is gathered related to maintaining or advancing EMSL capabilities or promoting EMSL.

Other Projects

EMSL staff should charge to projects that are not covered under EMSL's operations budget when they are asked to process routine samples or conduct experiments that solely and directly benefit a project not related to the operations of EMSL.

When determining whether staff time should be charged to the EMSL operations budget versus a user project, the individual should consider the amount of staff time the user requires. Submission of an EMSL User Proposal does not entitle the user to funding under the EMSL operations budget.

Examples of activities that should be charged to the user's project:

- Non-EMSL staff (e.g., from the Environmental Technology or National Security Directorates) request EMSL staff to run samples, perform analyses, or contribute to a report
- Non-EMSL staff request EMSL staff to travel to a conference to present information specific to one of the non-EMSL staff projects.

Points of Contact

The following individuals can assist with questions or provide further information:

Gregg Andrews	(509) 376-0231
Virginia Collier	(509) 372-3878
Cynthia Irwin	(509) 376-7422
Joy Rosscup	(509) 376-4263
Becky Wattenburger	(509) 376-4279

Appendix C — EMSL Space Occupancy Policy

To obtain office or laboratory space in the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), an individual must be engaged in the mission of EMSL. EMSL staff (organization code D7E2X) have the highest priority for occupancy, and occupancy for other research organizations and groups is evaluated annually for relevance to EMSL's mission.

In addition, certain support functions—as listed below—are essential to EMSL operations and thus are given high priority for space:

- Building Manager, power operators, facility engineers, and crafts resources
- Environment, Safety, Health and Quality staff
- Finance staff.

Other support staff who are considered for office space within EMSL on a low-priority basis include those from Economic Development and Communications and Contracts and Legal.

Support staff who are not to be housed in EMSL during office shortages include those from Human Resources and the DOE Richland Operations Office.

Office Space Loading Policy

Single-Person Offices

The following staff must be housed in single-person offices within EMSL and thus receive highest priority for those types of offices. In addition, those staff members who are connected to EMSL operations receive priority for the larger, single-person offices equipped with outer support staff space.

- EMSL Director
- EMSL Associate Directors
- Laboratory Fellows
- Battelle Fellows
- Technical Leads/Group Leaders.

The following staff may be assigned single-person offices, if available. Those staff members within this group who are not assigned laboratory space may receive priority for single-person offices in the following order:

- Job Evaluation System (JES) 40 and above
- Scientist and Engineer (S&E) 5
- S&E 4
- JES 30 to 39.

If no single-person offices are available, staff will be doubled according to the following order:

- JES 30 to 39
- S&E 4
- S&E 5
- JES 40 and above.

Double-Person Offices

Individuals who will be assigned double-person offices include S&E 1, 2, 3, or 4 staff (the latter depends on the lack of availability of single-person offices).

EMSL users, post-doctoral fellows, and students will be assigned double-person offices, as space permits; otherwise, they will be housed in triple-person or bullpen-style offices. Post-doctoral fellows should not be housed with EMSL staff unless those staff are of a junior level (i.e., S&E 1 or 2, Technician 1, 2, 3, or 4) and they work on the same projects.

Triple-Person and Bullpen-Style Offices

Individuals assigned to triple-person or bullpen-style offices include secretaries and clerks, students, technicians, post-doctoral fellows, users, and S&E 1 and 2.

Library/Collaboratory

Library/Collaboratory space is not designated for any particular research group but instead is assigned as needed. Criteria for use of space in these areas are similar to that outlined for triple-person or bullpen-style offices.

Additional Stipulations

Individuals who are currently housed in space where their job families exceed the criteria outlined in the EMSL space guidelines will not be removed unnecessarily to enforce conformance with policy; however, their office space is vulnerable to reassignment during the annual reassessment of EMSL mission relevancy.

Joint appointees from Washington State University who are performing long-term research at EMSL are treated as staff. Thus, if their research reflects EMSL's mission, office space is assigned accordingly.

Emeritus scientists are entitled to office space and are assigned space case by case relative to their status upon retirement and the frequency of office use.

Program requirements also drive occupancy priority. Staff members who are assigned laboratories or who provide support to laboratories in EMSL are given priority for office space as well.

EMSL makes every effort to provide an office or workstation to users and visitors on sabbatical, but makes no guarantees of actual assignment until additional office space is constructed.

Turnaround space within EMSL is the most vulnerable and is evaluated first when a need for additional office space arises.

Office and laboratory ownership of matrixed staff housed in EMSL is evaluated annually.

The office space needs of full-time staff supersede that needed by part-time and summer staff.

Laboratory Fellows may be placed in the larger offices in each pod (e.g., Rooms xx77, xx79, xx87, xx89). The xx75 offices are generally reserved for group leaders.

Implementation and Appeal

Any requests for office space should be directed to the EMSL space point-of-contact, Tobe Taylor. She will work with the requesting research group and the EMSL Operations Manager to identify space that will meet the individual's need.

Laboratories

Laboratory space may be requested from the EMSL Operations Manager. If space is available, the EMSL Operations Manager will evaluate proposed use to ensure that it aligns with EMSL's mission and whether the work will fit within the operating envelope of the facility. If these criteria are met, the EMSL Operations Manager will consult with both EMSL Associate Directors to authorize the space assignment.

If laboratory space is requested but no space is available, the EMSL Operations Manager will evaluate the value of the request against present use of EMSL space. If a laboratory is discovered to no longer house research in alignment with EMSL's mission or is significantly underused as demonstrated by resource use data, then the EMSL Operations Manager will work with the EMSL Director to render the final determination.