

**William R. Wiley
Environmental Molecular Sciences Laboratory**



The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), the U.S. Department of Energy's (DOE) newest national scientific user facility is located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research to facilitate multidisciplinary approaches to complex scientific and technical problems relevant to DOE missions and the nation's environmental challenges.

Capabilities in the EMSL include over 100 major instrument systems available to users, our resident research staff, and their collaborators. These capabilities are used to enable fundamental research on the physical, chemical, and biological processes that underpin critical environmental issues.

More information about EMSL capabilities and research programs is available on the EMSL web site.

<http://www.emsl.pnl.gov>

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Project information, software, user and developer help, presentations and references, contact information, and job/collaboration opportunities are available from our web site.

<http://collaboratory.pnl.gov>

**EMSL Research Instruments
Available to Remote Users via the Internet**



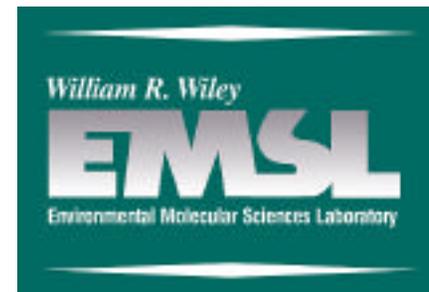
Molecular Science Computing Facility



Ion Trap Mass Spectrometer



High Field Magnetic Resonance Facility



**The EMSL Collaboratory
Scientific Collaboration
via the Internet**



**Pacific Northwest
National Laboratory**
Operated by Battelle for the
U.S. Department of Energy



The EMSL Collaboratory

The term "collaboratory" describes an ideal state in which computing and communications technologies render separations in time and distance meaningless to the collaborative pursuit of knowledge. Research groups form on a "just-in-time" basis and members share their instruments, data, software, publications, and expertise in a distributed virtual space that is as accessible as laboratories and offices down the hall. Collaboratories hold great promise in all fields of knowledge work including research, education, and information analysis. Use of collaboratories will improve the efficiency and effectiveness of researchers, their responsiveness to rapid changes, and their ability to handle complex research problems.

Researchers at the Pacific Northwest National Laboratory's Environmental Molecular Sciences Laboratory (EMSL) are developing and deploying a suite of technologies that will enable scientists to collaborate via the Internet. EMSL's researchers also are participants in the Department of Energy's multi-laboratory DOE2000 Collaboratory Project. The technologies developed in both the EMSL and DOE projects are helping users of pilot collaboratories at national scientific user facilities such as the EMSL to participate in experiment planning, data acquisition and analysis, report generation, and day-to-day discussions--all from different sites.

The Collaborative Research Environment

The Collaborative Research Environment (CORE2000) provides real-time access to data, software, research instruments, and expertise via the Internet. CORE2000 integrates technologies from the EMSL and its DOE2000 partners, the National Center for Supercomputing Applications (NCSA), and public domain technologies to provide access to:

- audio/video conferencing
- shared application display
- shared web browsing
- shared files
- remote controlled laboratory cameras
- collaborative instrument and analysis software.

Electronic Laboratory Notebook

Laboratory notebooks are primary repositories of scientific knowledge. An electronic notebook allows sharing of information across a distributed research group, thus enabling researchers to create and browse through plans, instrument diagrams, experiment parameters, graphs of data, and multimedia notes. EMSL researchers are working with their DOE2000 partners to build a secure, extensible, web-based system that provides these capabilities.

Developing EMSL Virtual Facilities

A growing number of the EMSL's scientific resources are being made remotely accessible, including mass spectrometers (EMSL Online Project), nuclear magnetic resonance spectrometers, (Virtual NMR Facility Project), computational chemistry software (NWChem), and the 512-node IBM SP supercomputer (Molecular Science Computing Facility). EMSL's general compute and data storage resources also are remotely accessible. Access to these resources, combined with the capabilities of CORE2000 and the electronic notebook, make it possible for researchers to directly participate in many aspects of experiments conducted in EMSL laboratories without having to leave their home institutions. Today, more than 25 percent of the external researchers using EMSL nuclear magnetic resonance spectrometers do so via the Internet. Using the published programming interfaces of the DOE2000 tools, new capabilities can be woven into custom virtual facilities. Data acquisition, analysis, visualization, and modeling tools can be linked with CORE2000 to allow group control of these applications and to support real-time consultation and training while experiments are being run. Applications also can be linked directly to the electronic notebook, allowing researchers to save data directly into shared notebooks as easily as saving to a local disk. Notebook extensions allow the development of custom Spectroscopists' Notebooks in which mass spectra are shown as live, zoomable graphs, and protein geometries appear as three-dimensional structures that can be rotated for viewing from different perspectives.

Support for EMSL Users

The successful introduction of Collaboratory-style interactions into a major scientific user facility such as the EMSL requires operations support as well as developmental efforts. EMSL staff are developing, integrating, and deploying a wide variety of technologies to support remote access. The EMSL accepts research proposals via its web site on the World Wide Web. Instrument capabilities and schedules are available online. Collaborative tools are supported with automated registration, commercial installation packages, WWW-based support queues, and email discussion lists. Monitoring software verifies the operational status of collaborative services and tracks usage. Usage statistics and interviews with users contribute to our understanding of distributed group dynamics and help refine strategies for tool development and organizational deployment.

Collaborations

In addition to DOE2000 related partnerships with other national laboratories (Argonne, Lawrence Berkeley, Oak Ridge, and Sandia) and with NCSA, EMSL has a wide range of collaborations that focus on the development and use of collaborative technologies for research and education. EMSL has formal agreements with the Collaborative Electronic Notebook Systems Association, an industry group that promotes the use electronic notebooks, and with the Alliance for the Advancement of Science through Astronomy, a nonprofit corporation that is bringing the Rattlesnake Mountain Observatory in eastern Washington online. EMSL Collaboratory researchers also work with individual groups of faculty, staff, and students at a variety of colleges and universities.

Software Availability

CORE2000 and the Electronic Laboratory Notebook are publicly available from the EMSL web site. Project information, developer kits, user and developer help, presentations and literature citations, contact information, and collaboration/job opportunities are also available.

<http://collaboratory.pnl.gov>