

William R. Wiley
Environmental Molecular Sciences Facility



The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility. EMSL is the centerpiece of DOE's commitment to provide world-class research capabilities for enabling fundamental research on the physical, chemical, and biological processes that underpin critical scientific issues.

EMSL capabilities are used to address the fundamental science that will be the basis for finding solutions to national environmental issues such as cleaning up contaminated areas at DOE sites across the country and developing "green" technologies to reduce or eliminate future pollution production. The capabilities also are used to further our understanding of global climate change, environmental issues relevant to energy production and use, and health effects resulting from exposure to contaminated environments.

If you are interested in collaborating with our scientists or using the facility's resources, more information and specific procedures for becoming an EMSL user and proposal details can be found at our web site
<http://www.emsl.pnl.gov>.

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Related Web Sites

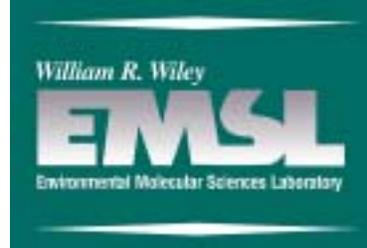
MSCF
<http://mscf.emsl.pnl.gov>

MS³
<http://mscf.emsl.pnl.gov/capabs/mscf/software/ms3.html>

Ecce
<http://www.emsl.pnl.gov/pub/docs/ecce>

NWChem
<http://www.emsl.pnl.gov/pub/docs/nwchem>

ParSoft
<http://www.emsl.pnl.gov/pub/docs/parsoft>



Molecular Science Computing Facility



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



Molecular Science Computing Facility

The Molecular Science Computing Facility (MSCF) provides the advanced computing capability of the William R. Wiley Environmental Molecular Sciences Laboratory to address "Grand Challenge" scale environmental research problems of the U.S. Department of Energy (DOE). The MSCF has an integrated production computing environment, with links to external facilities within DOE, collaborating universities, and industry.

Interconnections at EMSL feature fiber-to-the-desktop, with multiple pairs of multimode and single mode fibers throughout the facility, connecting to a hierarchy of flexible network equipment in the MSCF. Standard services include 10 and 100 Mbts switched Ethernet. Gigabit Ethernet is available throughout the facility for computing equipment with high speed network requirements.

Resources include a High Performance Computing Center, Experimental Computing Laboratory, Graphics and Visualization Laboratory, and next-generation software for parallel high performance computing systems.



Graphics & Visualization Laboratory

High Performance Computing Center contains a new Hewlett Packard Linux-based computer for production and testing, as well as a high performance 40-terabyte disk archive system. With a theoretical performance of 1 Tflop, the primary production system has 128 nodes/



256 Itanium-2 processors, 1.5 TB of memory, and 40 TB disks. This is phase 1 of the continual upgrade to a 11+ Tflops, 1900+ processors system in 2003.

High Performance Computing Center

Experimental Computing Laboratory contains a 240 processor Dell Linux cluster and a small HP cluster with the next generation processor. These systems provide the MSCF strategic software research and development teams with innovative computer systems that help reduce simulation costs.

Graphics & Visualization Laboratory provides in-house production facilities for the display and analysis of large complex data sets from both experiments and simulations. The GVL contains 2 high-performance 8 node SGI graphics servers, an IBM Scalable Graphics Engine for parallel graphics, and a small 8 processor Dell Linux cluster. A digital audio/video editing system to facilitate the display and capture of scientific visualization.

Molecular Science Software Suite MS³ is a unique, comprehensive, and integrated suite of software that enables computational chemists to focus their advanced techniques on finding solutions to complex issues involving chemical systems. MS³ is composed of the Extensible Computational Chemistry Environment – Ecce, the Northwest Computational Chemistry Software – NWChem, and the Parallel Software Developments Tools – ParSoft.

Developed at the EMSL, MS³ won the R&D Magazine R&D 100 Award in 1999 and the Federal Laboratory Consortium Award for Technology Transfer in 2000.

Operations Management works to ensure that computational resources are continuously and efficiently made available to the Grand Challenge and other MSCF scientific projects. Innovative solutions are crafted to address challenges arising from High Performance Computing in areas such as parallel I/O, scheduling, security, and accounting.

In order to fairly distribute computing resources to various users and projects, an allocation management tool called QBank. QBank associates a cost per resource and dynamically charges the project for their utilization of the system, thus providing full accounting of each resource used.

