

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 can be found at <http://www.emsl.pnl.gov>.

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## Related Web Sites

### MSCF

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

### MS<sup>3</sup>

<http://mscf.emsl.pnl.gov/software/ms3.shtml>

### Ecce

<http://ecce.emsl.pnl.gov/index.shtml>

### NWChem

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

### ParSoft

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

# Molecular Science Computing Facility



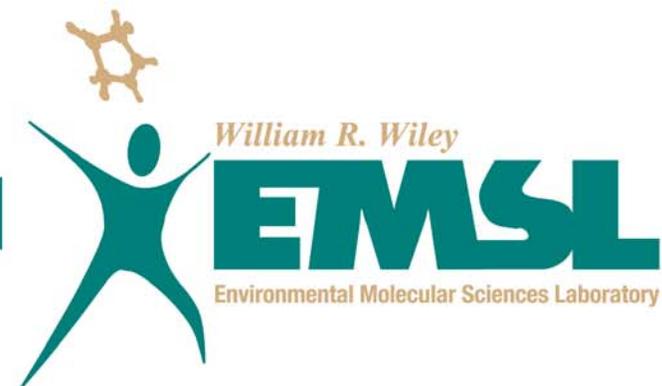
[www.emsl.pnl.gov](http://www.emsl.pnl.gov)

The W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research.

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



Office of  
Science  
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 Mbps 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 & 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 disk archive system. With a theoretical performance of over 11 Tflops, the primary production system has 980 nodes/1,960 Itanium-2 processors, 6.8 TB of memory, and roughly a half of a petabyte of disk. This system became fully operational during 2003 and is one of the fastest supercomputers in the world.



*High Performance Computing Center.*

## Experimental Computing Laboratory

contains a variety of new and exciting computer architectures. 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 a high performance 8-node SGI graphics server, a 16-processor Linux cluster with an IBM Scalable Graphics Engine (SGE3) for parallel graphics, and 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 Gold has been developed. Gold associates a cost per resource and dynamically charges the project for their utilization of the system, thus providing full accounting of each resource used.



*Operations Management.*