

William R. Wiley

EMSL

Environmental Molecular Sciences Laboratory

The W.R. Wiley Environmental Molecular Sciences Laboratory, a national scientific user facility at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of the U.S. Department of Energy and the nation.

Through its mission, EMSL staff and capabilities enable multidisciplinary approaches to complex scientific problems and provide a climate for advancement and education in the molecular and computational sciences. The user facility offers the research community, at one location, a comprehensive array of leading-edge resources available to users on a peer-reviewed proposal basis.

To submit a proposal for use of EMSL or to learn more about the science conducted at EMSL and the instruments and expertise available to users, visit <http://www.emsl.pnl.gov>. If you have any questions, please contact EMSL User Services at emsl@pnl.gov.

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Molecular Science Computing Facility



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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 DOE Office of Biological and Environmental Research.

Pacific Northwest
National Laboratory
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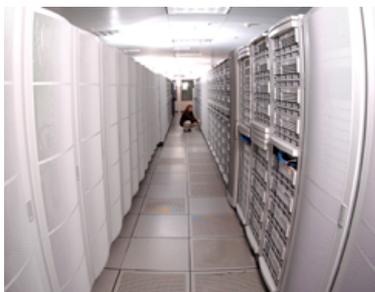
Molecular Science Computing Facility

The Molecular Science Computing Facility (MSCF) provides the advanced computing capability of the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) 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.

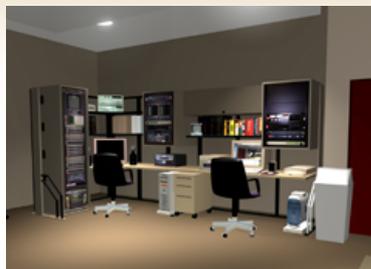
Interconnections at EMSL feature fiber-to-the-desktop, with multiple pairs of multimode and single mode fibers throughout the facility, connecting to a hierarchy of flexible network equipment in the MSCF. Standard services include 100 Mbts switched Ethernet with 1 Gbt available, if needed. Gigabit Ethernet is available throughout the facility for computing equipment with high-speed network requirements.

High-Performance Computing Center

contains a 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 teraflops, the primary production system has 980 nodes/1960 Itanium-2 processors, 9.7 terabytes 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.



Graphics & Visualization Laboratory



provides in-house production facilities for the display and analysis of large complex data sets from both experiments and simulations. It contains a high-performance 16-node SGI graphics server, a 16-processor Linux cluster, and a digital audio/video editing system to facilitate the display and capture of scientific visualization. Printers are available for printing posters, and a digital printer with high-definition format capabilities can be used for photo-quality prints. Several workstations are also available for training and visitors.

Molecular Science Software Suite

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 (Global Array Tools).

Developed at 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 distribute computing resources fairly to various users and projects, an allocation management tool called Gold has been developed. Gold associates a cost per resource and dynamically charges projects for their utilization of the system, thus providing full accounting of each resource used.



NWfs—Data Archiving System

is a disk-based archive system, with commodity components and the Lustre file system, which was developed to address EMSL's growing data storage and access needs. NWfs is the first storage system of its type in a supercomputing environment. It is comprised of a clustered storage server configuration, with each server containing 4 terabytes or more of disk space. The Lustre file system aggregates the storage on all individual servers, providing a single, very large storage pool. Currently, the system provides 300 terabytes of disk space and is ultimately expected to grow to the petabyte (1000 terabyte) range.

Related Web Sites

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

MS³: <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>

Global Arrays:
<http://www.emsl.pnl.gov/docs/global>

Basis Set Library:
http://mscf.emsl.pnl.gov/software/basis_intro.shtml