

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

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

Ecce
<http://ecce.emsl.pnl.gov>

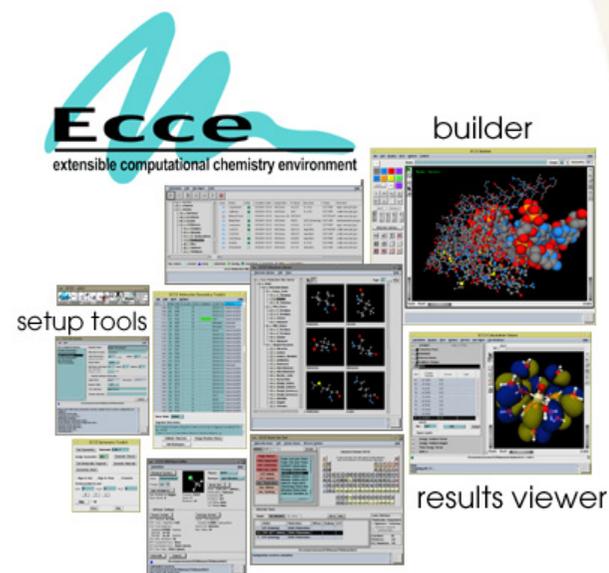
Awards

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



Gaussian is a trademark of Gaussian, Inc.; LSF is a trademark of Platform Computing; Sun Grid Engine is a trademark of Sun Microsystems; NQE and NQS are trademarks of Cray, Inc.; LoadLeveler is a trademark of IBM

Extensible Computational Chemistry Environment



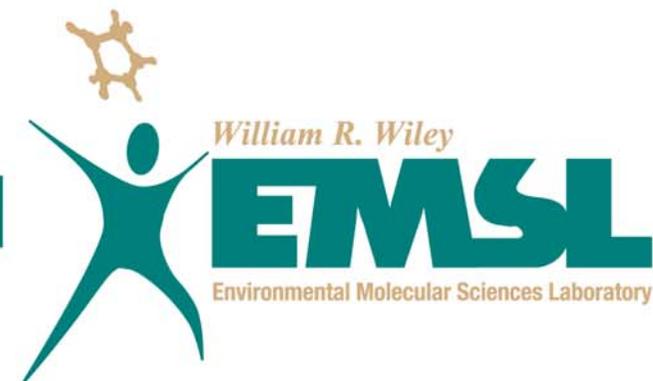
www.emsl.pnl.gov

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



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Science
U.S. DEPARTMENT OF ENERGY



Ecce

Extensible Computational Chemistry Environment

The Extensible Computational Chemistry Environment (Ecce) is a domain encompassing problem-solving environment for computational chemistry. Ecce is composed of a suite of distributed client/server UNIX based graphical user interface applications seamlessly integrated together. The resulting environment enables research scientists to transparently utilize complex computational modeling software accessing high-performance compute resources from their desktop workstations.

The Ecce software architecture is based on an object-oriented chemistry data model to support the management of computational and experimental molecular data. The Ecce team has developed a flexible high-performance data management component built on Web technologies and the Extensible Markup Language (XML) for data interchange and storage. The environment is built for extensibility to support new computational codes and capabilities through script files for managing both code input and output rather than reworking the core applications.

The Ecce application software currently runs on Linux, SGI, and Sun workstations and is written in C++ using the X Window System Motif user interface toolkit and OpenGL graphics. Ecce provides a sophisticated user interface, scientific visualization tools, and the underlying data management framework to enable scientists to efficiently set up calculations and store, retrieve, and analyze the rapidly growing volumes of data produced by computational chemistry studies.

General Features

- Support for building molecular models
 - Three-dimensional direct manipulation builder
 - Symmetry building operations and symmetry recognition
 - Manipulation and preparation of large systems for molecular dynamics simulations
 - Import and export of structures in a variety of standard file formats
 - Extensive multi-step undo capability
 - Many preloaded structures, including all standard biological residues, in a Structure Library
 - User created libraries of molecular structures
 - Builder available as a separate, standalone application
- Graphical user interface to a broad range of electronic structure theory types. Supported codes currently are NWChem, Gaussian 98™, and Amica. Other codes will be registered based on user requirements.
- Graphical user interface for basis set selection
 - Over 230 basis sets are currently contained in the Basis Set Library
 - Basis set coverage can be specified for overall structure or on an element-by-element basis
 - Exponents, coefficients, detailed reference and citation information is available for each basis set
 - Export of basis sets to several computational code file formats is possible.
- Remote submission of calculations to UNIX and Linux workstations, clusters, and supercomputers running LSF™, PBS, NQE/NQS™, Sun Grid Engine™,

LoadLeveler™, and Maui Scheduler is supported.

- Remote communications are handled using the standard protocols secure shell and copy (ssh/scp), telnet/ftp, remote shell and copy (rsh/rcp), and Globus (developed by Argonne National Laboratory).
- No installation beyond the computational code is required on the remote compute servers (including no requirement for a "root" daemon).
- Includes support for importing results from NWChem, Gaussian 94™, and Gaussian 98™ calculations run outside of the Ecce environment.
- Three-dimensional visualization and graphical display of molecular data properties while jobs are running and after completion. Supported properties include vibrational frequencies, molecular orbitals, electrostatic potentials, spin and electron densities, dipole and quadrupole moments, mulliken charges, NMR shielding coefficients, geometry optimization steps, energies, and molecular dynamics trajectories.
- Extensive web based help. See <http://ecce.emsl.pnl.gov/help>

Future Research & Development

Ongoing development is extending Ecce to support the setup and analysis of molecular dynamics simulations and specifically the NWChem MD module. External collaborations with computational chemists are resulting in new codes being integrated into Ecce. Advances in the design and development of problem-solving environments pioneered by Ecce serve as a foundation for new PNNL and collaborative projects within and beyond computational chemistry.