



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>



The Molecular Science Software Suite (MS³) was developed at Pacific Northwest National Laboratory. In 1999, MS³ was recognized by *R&D Magazine* as one of the top 100 technologically significant and new processes of the year, and in 2000, it received a Federal Laboratory Consortium Award for Technology Transfer..

More information about MS³ and its three components, *Ecce*, *NWChem*, and *ParSoft*, are provided in this brochure and on the World Wide Web.

MS³

<http://www.emsl.pnl.gov/pub/capabs/mscf/showcase/ms3-1999.html>

Ecce

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

NWChem

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

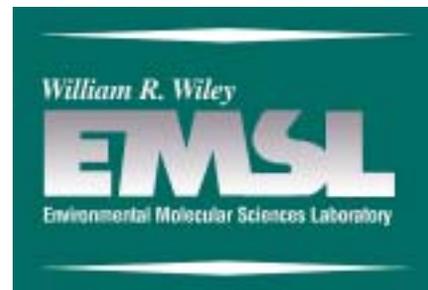
ParSoft

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

For additional information, contact:

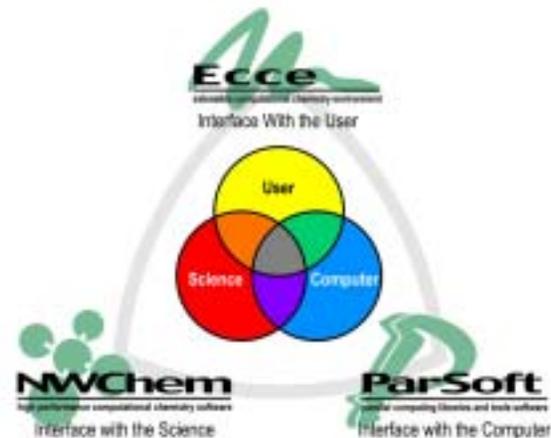
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MS³

Molecular Science Software Suite



Pacific Northwest
National Laboratory

Operated by Battelle for the
U.S. Department of Energy



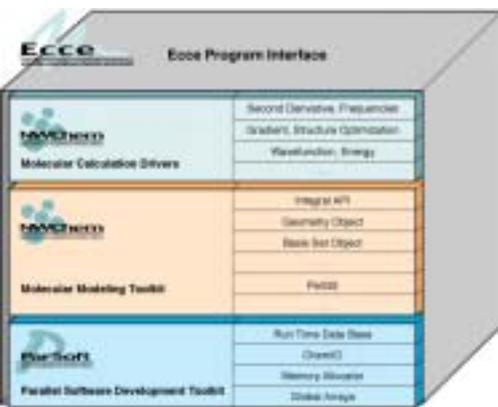
Molecular Science Software Suite

The 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. It is the first general purpose collection of software that provides access to high-performance, massively parallel computers for chemists with a broad range of applications.

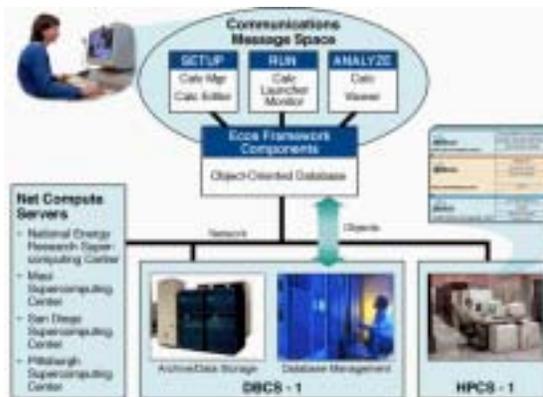
MS³ is composed of the Extensible Computational Chemistry Environment -- *Ecce*, the Northwest Computational Chemistry Software -- *NWChem*, and the Parallel Software Development Tools -- *ParSoft*.

Although many of the features of MS³ are available piecemeal in other codes, it is the first truly integrated computational chemistry software system for massively parallel computers to provide a single platform from which to run quantum mechanics calculations, molecular dynamics, and data analysis and visualization.

MS³ was developed to support the modeling and simulation of chemical systems relevant to U.S. Department of Energy environmental clean-up efforts and other national issues.



MS³ Infrastructure



Ecce-NWChem-ParSoft -- Distributed Client/Server Model

Principal Applications of MS³

MS³ is currently in use at many of the national supercomputer centers, national laboratories, and universities. These are not just single users in most cases but are actually large computer divisions. Calculations performed with the software include studies of

- protein models for drug design
- geochemical surfaces for bioremediation
- systems to separate radioactive metal ions
- actinide-complex contaminants
- petrochemical zeolite catalysts
- reactions in aqueous solutions
- atmospheric aerosol pollutants
- combustion simulation.

There are an enormous number of potential applications for MS³ as new, faster, and more powerful high-performance computer systems are developed. Examples include

- prediction of biological activity
- environmental impact studies
- catalyst design
- materials design.

MS³ Components

Ecce provides an integrated environment for distributed client/server applications, thus enabling scientists to easily use computational software such as *NWChem* by accessing networked high-performance computers from their desk-top workstations. Using graphical user interface (GUI) tools, *Ecce* allows scientists to compose structures and data input and then initiate the calculations. Results are stored for further analysis and are readily accessed from *Ecce*.

NWChem is a high-performance molecular modeling software package. It is capable of computing the electronic structures of molecules and periodic systems for extremely large structures. *NWChem* can implement SCF, DFT, and higher order calculations, and it has molecular dynamic potentials that support classical mechanics calculations. *NWChem* will determine energies, optimized geometries, gradients, and other properties, and it can perform molecular dynamics simulations and normal mode analyses. Molecular dynamics simulations have been performed on 200,000-atom systems, and quantum mechanical properties have been determined for compounds up to 1,000 atoms.

ParSoft provides the efficient and portable computing libraries and tools that enable the user to run on a wide variety of parallel computing systems with leading-edge performance and scalability. Originally developed to run on the IBM SP computer, MS³ has since been ported to other systems, including the Cray T3D and T3E, the Intel Paragon, the Silicon Graphics Origin 2000, and clusters of workstations.



IBM SP in the Molecular Science Computing Facility