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 can be found at our web site http://www.emsl.pnl.gov.

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Related Web Sites

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

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

Awards

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

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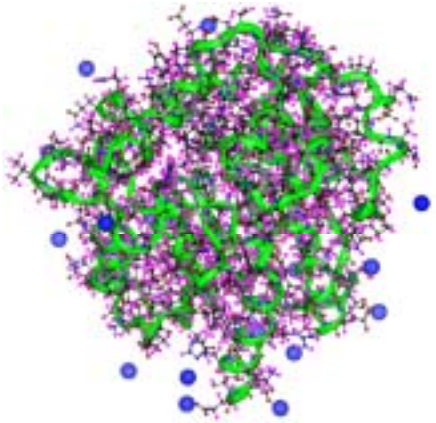
NWChem

High Performance
Computational Chemistry



Pacific Northwest
National Laboratory
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NWChem

High Performance Computational Chemistry

The High Performance Computational Chemistry group in the Environmental Molecular Sciences Laboratory's Theory, Modeling, and Simulation program focuses on developing next generation molecular modeling software for massively parallel computers. The group applies the software in testing and benchmarking of new capabilities and investigation of problems relevant to DOE.

Our development of efficient implementations of advanced molecular methods is targeted to the high performance parallel computer systems installed in the Molecular Science Computing Facility (MSCF) and the emerging teraflops class of massively parallel computers. Key aspects are recasting algorithms and creating new approaches for expressing the fundamental physics involved. Thus, there is need for theoretical and computational innovation, especially as we tackle longer length and time-scales and higher levels of accuracy.

We have also emphasized making parallel programs easier to write, maintain, and extend. NWChem readily interfaces with other program suites, such as the natural bond orbital (NBO) package, POLYRATE, and Python, in order to leverage existing functionality and to make our unique functionality readily accessible to others.

NWChem is designed to be scalable with both problem and machine size, and to be highly portable, making it available for almost all high performance computing platforms or workgroup servers. Efforts have been devoted to providing maximum efficiency on massively parallel processors such as the 512-node IBM SP system in the MSCF and the 512-node CRAY T3E system at the National Energy Research Scientific Computing Center (LBNL). NWChem includes the following methods:

Molecular Electronic Structure

For energies and analytic first derivatives with respect to atomic coordinates: 1) Hartree-Fock (RHF, UHF, high-spin ROHF), 2) Gaussian orbital based density functional theory (DFT) using many local and non-local exchange-correlation potentials (LDA and LSDA), 3) semi-direct MP2 using frozen core and RHF and UHF references, and 4) complete active space SCF.

These methods are available to compute energies only: 1) CCSD(T) with RHF reference, 2) MP2 fully direct with RHF reference, 3) selected CI with second-order perturbation correction, and 4) resolution of the identity integral approximation MP2 (RI-MP2) with RHF and UHF references.

For all methods the following may be performed: 1) single point energy, 2) geometry optimization with constraints (minimization and transition state), 3) molecular dynamics on the fully ab initio potential energy surface, 4) numerical first and second derivatives automatically computed if analytic derivatives are not available, 5) normal mode vibrational analysis in Cartesian coordinates, 6) ONIOM, 7) COSMO, 8) evaluation of static, one-electron properties, and 9) electrostatic potential fit of atomic partial charges.

Periodic System Electronic Structure

A Gaussian Approach to Polymers, Surfaces, and Solids (GAPSS) is available to compute energies and gradients by periodic Gaussian-based DFT with many local and non-local exchange-correlation potentials.

Molecular Dynamics

Classical molecular simulation functionality includes 1) single configuration energy evaluation, 2) energy minimization, 3) molecular dynamics simulation, and 4) free energy simulation (MCTI and MSTP with single or dual topologies, double wide sampling and separation-shifted scaling).

Classical and quantum descriptions may be combined to perform 1) mixed quantum mechanics molecular dynamics simulation and molecular mechanics energy minimization, 2) quantum molecular dynamics simulation by using any of the quantum mechanical methods capable of returning gradients.

The classical force field includes 1) effective pair potentials, 2) first-order polarization, 3) self consistent polarization, 4) smooth particle mesh Ewald, 5) twin range energy and force evaluation, 6) periodic boundary conditions, 7) SHAKE constraints, and 8) contant temperature and/or pressure ensembles.

Pseudopotential Plane-Wave Electronic Structure

These modules are available to compute the energy, minimize the geometry, and perform ab initio molecular dynamics using pseudo-potential plane-wave DFT with local exchange-correlation potentials: 1) fixed step length steepest descent and 2) Car-Parrinello (extended Lagrangian dynamics). This capability comes with 1) LDA and LSDA exchange-correlation potentials, 2) (Γ–Point) periodic orthorhombic simulation cells, 3) Hamann and Troullier-Martins norm-conserving pseudopotentials, and 4) modules to convert between small and large plane-wave expansions.