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EMSL In Brief
Environmental Molecular Sciences Laboratory

NWChem, Version 5.1, Now Available

EMSL offers updated, more powerful computational chemistry software

Developed by the experts at the Environmental Molecular Sciences Laboratory, the latest version of NWChem is now available. Working on either parallel supercomputers or on workstation clusters, NWChem applies theoretical techniques to predict the structure, properties, and reactivity of chemical and biological species, ranging in size from tens to millions of atoms. The new version, NWChem 5.1, provides the following capabilities:

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

Available on latest platforms. NWChem has been ported to the IBM BlueGene/L and the Cray-XT3/XT4 platform, with computational scalability of up to at least 1024 processors on both. In addition, NWChem now supports Infiniband/OpenIB network.

New accurate energetics and properties calculations. In NWChem, a coupled-cluster linear response is now available using both restricted and unrestricted references. Ground-state dynamic polarizabilities at the coupled-cluster singles, doubles, and triples levels of theory are now available. Second-order approximate coupled-cluster model with singles and doubles (CC2) is available for excited states. In addition, performance improvements have been made in both time-to-solution and memory usage.

Better modeling of heavy element chemistry. The new spin-orbit zeroth-order relativistic approximation is available in both the Gaussian and plane wave density functional theory modules, providing a framework for heavy element chemistry simulations. In addition, the spin-orbit Douglas-Kroll approach is now available.

New science possible with plane wave module. Users of NWChem's plane wave code can now use Fermi smearing to model metals. In addition, the plane wave module can now handle any general pseudopotential, and performance improvements enable a faster time to solution and improved scalability.

Users contribute new capabilities to NWChem. The constrained density functional theory method developed by the Van Voorhis Group is now available. In addition, the Truhlar Group has made their latest M06 density functional available in NWChem.

Subject to the terms and conditions of the software user agreement, NWChem is available free of charge. See http://www.emsl.pnl.gov/docs/nwchem/nwchem.html

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