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EMSL In Brief

Environmental Molecular Sciences Laboratory

EMSL Releases NWChem Version 5.0

Software developers at the Environmental Molecular Sciences Laboratory (EMSL) have released a new version of the premier computational chemistry software, NWChem. NWChem has long provided a scalable software tool that allows users to study large scientific computational chemistry problems efficiently using parallel computing resources, from high-performance supercomputers to conventional workstation clusters. Some of the new capabilities available with NWChem Version 5.0 include the following:



NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL
CHEMISTRY SOFTWARE

- Improvements and optimizations have resulted in a much faster time-to-solution in the high-accuracy TCE and CCSD(T) codes, which enables users to address scientific problem sizes that could not be addressed before.
- The quantum mechanics/molecular mechanics module provides seamless integration between molecular mechanics and most quantum-mechanical theories and properties.
- Equation of Motion CCSD(T), combined with completely renormalized techniques, provides an ideal framework for large-scale calculations of singly and partially doubly-excited states.
- The NWChem plane-wave module now enables users to use exact exchange and the Self-Interaction Correction within its framework for complex molecular, liquid, and solid-state systems.
- The molecular dynamics module now includes the capability for dynamic proton hopping using the new, efficient Q-HOP methodology developed at the University of Saarland, Germany.
- Interface capabilities with VENUS—a general chemical dynamics program developed by Texas Tech University—enable users to study chemical reactions through classical chemical dynamics simulations.

NWChem, part of EMSL's award-winning Molecular Science Software Suite, has been distributed to more than 1400 sites worldwide. Details about NWChem, including a user's guide and download information, are located at <http://www.emsl.pnl.gov/docs/nwchem/nwchem.html>. For more information, contact Bert de Jong (509-376-5290).

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