

NWChem: Pushing the scientific envelope on large computing platforms

W. A. de Jong

Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Mail stop K8-91, P.O. Box 999, Richland, WA, 99352.

With the emergence of computing platforms that are a hundred teraflops, and with petascale computing platforms on the horizon, computational chemistry (and computational chemistry software) is on the verge of entering a new era of modeling. These huge computing resources will enable researchers to tackle scientific problems that are larger and more realistic than ever before, and to include more of the complex dynamical behavior of nature. In this presentation we will discuss the extensive suite of capabilities available in NWChem, and the scalability of the software on large scale computing platforms. NWChem is DOE's premier quantum chemistry software developed at the Environmental Molecular Science Laboratory at Pacific Northwest National Laboratory, and is freely available to the scientific community.

This work was supported through the U.S. Department of Energy by the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory. The EMSL is funded by the Office of Biological and Environmental Research in the U.S. Department of Energy. Pacific Northwest National Laboratory is operated by Battelle Memorial Institute for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830.