Upgrades to NRLMOL code

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NRLMOL, the Naval Research Laboratory Molecular Orbital Library is a massively parallel code for electronic structure calculations on large molecules and clusters. The code is based on Kohn-Sham formulation of density functional theory and solves Kohn-Sham equations by expressing the Kohn-Sham orbitals as a linear combination of Gaussian orbitals. It permits full or partial structure optimization, calculations of harmonic vibrational frequencies, infra-red spectra, Raman spectra, polarizability, density of states, joint density of states, vibrational polarizability etc. NRLMOL uses the point group symmetry of molecules in efficient manner, and practically any point group (e.g. D20H, Ih, C40H etc) can be used. The default basis set of the NRLMOL has been specifically optimized for the PBE exchange-correlation functional and is much larger than the default basis sets used in other codes.

The presented work is a series of upgrades that expand the computing capabilities of the code to allow it to simulate larger systems and reduce execution time by making use of recent advances in programming languages and computational mathematical libraries. The use of advanced MPI programming techniques will be presented, as well as memory management,ScaLAPACK, OpenMP and BLAS implementations.

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Event:MS Thesis defense
Date: Thursday December 20,2012
Time: 2:00pm
Location: Physical Science Building room 222