ACES III: Parallel Implementation of Electronic Structure Energy, Gradient and Hessian Calculations

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December 6, 2007

Abstract

Several computationally demanding components of the computational chemistry code ACES II have been completely redesigned and implemented in parallel. The design uses an extreme form of object-oriented programming. The high level algorithms are: Hartree-Fock (HF) self consistent field (SCF), seond-order many-body perturbation (MBPT(2)) energy, gradient, and hessian and couples-cluster singles, doubles and perturbative triples (CCSD(T) energy and gradient. For SCF, MBPT(2) and CCSD(T) both restricted Hartee-Fock (RHF) and unrestricted Hartree-Fock (UHF) reference wave functions are available. For MBPT(2) gradients and Hessians a restricted open-shell Hartee-Fock (ROHF) reference is also supported. The methods are programmed in a special language designed for the parallelization project. The language is called super instruction assembly language (SIAL). All compute intensive operations, such as tensor contractions, diagonalizations, ect, and all input-output operations are handled by a parallel program written in C and Fortan 77. This parallel program reads and executes the SIAL program and is called the super instruction processor (SIP). By separating the algorithmic complexity (in the SIAL) from the complexities of execution on computer hardware (in the SIP), a software system is created that allows for very effective optimization and tuning on different hardware architectures with quite manageable effort.

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