

**Parallel Implementation of Reduced Scaling Coupled Cluster Methods
and Experiences with the
Common Component Architecture in Quantum Chemistry**

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It is widely recognized that the high-order scaling with respect to molecular size of accurate electronic structure theories is both nonphysical and a severe impediment to their widespread application. Reformulated versions of these methods that scale less dramatically, ideally linearly with the system size, have been developed. These methods still have a significant computational cost, however, and their application to many systems of interest in biology or nanotechnology requires the use of parallel computing. We describe a parallel implementation of reduced scaling local coupled-cluster methods within the framework of the Massively Parallel Quantum Chemistry (MPQC) program.

We are also involved in an effort to provide standardized interfaces to quantum chemistry codes using the Common Component Architecture (CCA). This allows others to develop applications dependent on quantum chemistry methods without being concerned with the details of one particular package, as well as, more powerfully, combine several components into a single application. We will discuss our experiences with the CCA, and present benchmarks showing the performance impact.