Massively Parallel Implementation of MRD-CI

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We report on a scalable implementation of the configuration-selecting multi-reference configuration interaction method for massively parallel architectures with distributed memory. Based on a residue driven evaluation of the matrix elements this approach a llows the routine treatment of Hilbert spaces of up to ten billion determinants. We demonstrate the scalability and performance of the method for up to 128 nodes on the IBM-SP2 and for up to 256 nodes on the CRAY-T3E.
In addition to the methodology we will present initial applications of this code for ground- and excited state calculations that require a balanced treatment of dynamical and non-dynamical correlation effects, and possibly the inclusion of triple- and quadruple- excitations, in large basis sets.