Integral direct and memory conservative CCSD residual algorithm

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A novel implementation for the coupled cluster singles and doubles (CCSD) vector equations is presented. The algorithm is designed for low memory consumption and moreover it is efficiently parallelizable for several nodes. The recently developed divide-expand-consolidate (DEC) method is a linear scaling approach for coupled cluster methods, taking the local character of correlation into full account. In this approach the calculation is split into independent fragment calculations and the precision is determined by only one single input threshold, the fragment-optimization-threshold (FOT). Given that the fragments do not exceed a certain size the presented algorithm is suitable for large scale calculations of coupled cluster energies on large supercomputer systems. Hereby the time to solution will be drastically reduced compared to standard implementations. It will be shown how the presented algorithm performs compared to convenient implementations and how it is used within the DEC method. A further step of parallelization can be introduced by employing parallel distributed memory, which reduces the calculation time and broadens the range of application for the algorithm, since larger fragments and larger basis sets can be treated.