

The Divide-Expand-Consolidate DEC coupled cluster (CC) model: A black box linear-scaling approach with correlation energy-based error control

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We describe the Divide-Expand-Consolidate (DEC) coupled cluster (CC) model [1], where a full HartreeFock reference CC calculation on a molecular system is carried out in terms of CC calculations on small orbital fragments of the total molecular system. The orbital fragmentation does not involve physical bond cuts or a priori assignments of local orbital spaces. Rather it involves a splitting of the correlation energy into orbital fragment contributions where the sizes of the orbital fragment spaces are determined in a black box manner to ensure that the CC correlation energy is calculated to a preset energy threshold. This is possible because the least-change molecular (LCM) basis is employed, where both occupied and virtual orbitals are local. The number of independent fragment calculations scales linearly with the system size, making the method linearly scaling and embarrassingly parallelizable. We present a thorough locality analysis of the amplitude equations for second order Møller-Plesset perturbation theory (MP2) and the coupled cluster singles doubles (CCSD) model, which demonstrate that the amplitude equations are indeed local when expressed in the LCM basis. The locality analysis is supported by numerical results.

- [1] M. Ziolkowski, B. Jansík, T. Kjærgaard and P. Jørgensen *J.Chem.Phys*, **133**, 014107 (2010)