ABSTRACT

The divide-expand-consolidate local coupled cluster CCSD(T) model.

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It will be described how the Divide-Expand-Consolidate (DEC) strategy that previously has been applied to MP2 and CCSD can also be applied to CCSD(T) leading to a linear scaling and embarrassingly parallel algorithm. Numerical examples will be given to demonstrate the error control that may be imposed on the precision of the correlation energy through the fragment optimization threshold (FOT) parameter. This brings the DEC strategy on par with standard implementations where the parameter representing the threshold for the residual norm of the amplitude equations impose the error control on the correlation energy.