On the usage of local orbitals for approximated Coupled Cluster Methods

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While Coupled Cluster (CC) methods are the first choice of *ab-initio* methods when results of high accuracy are required, the high scaling of computational effort with molecular size prohibits their application to larger systems. Recent years have witnessed the development of various approaches for approximated CC methods to overcome this bottleneck.
Most of these methods make use of localized orbitals of one kind or another, prominent examples are the LCC methods presented by Werner, Schuetz et. al. [1] based on ideas by Saebøand Pulay [2] that use Pipek-Mezey [3] orbitals, the AO based Brueckner CCD algorithm described by Scuseria and Ayala [4] and approximations like the DIM and TRIM approach by Head-Gordon et. al. [5] which is based on so-called EPAOs [6]. However, as most of these methods are based on a certain kind of orbitals, no investigations using different types of orbitals in the framework of the same approximation have been carried out so far to the best of our knowledge.
In the dynamical thresholding CC approach [7] local energy contributions are calculated at the MP2 level and the size of each contribution is used as a screening criterion for the evaluation of the Coupled Cluster amplitudes. This leads to a systematical hierarchy of approximations with a threshold driven control of the accuracy. Furthermore, the present test implementation is not dependent on the specific choice of a certain set of local orbitals. Thus, the influence of the choice of the local basis can be investigated on the same footing. The truncation error and the number of discarded contributions can be monitored using for example the nonorthogonal, overcomplete pure AOs or Enveloping Localized Orbitals (ELOs) [7] , the orthogonal Pipek-Mezey orbitals or the nonorthogonal Projected AOs.
In this presentation we apply the dynamical thresholding CC approximation using a variety of different local orbitals (occupied and virtual) in order to investigate the wavefunction parameter sparsity and the resulting truncation error.

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