Efficient Implementation of Highly Excited Coupled Cluster

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We present recent advances of our coupled cluster implementation, which can treat in principle arbitrary excitation levels. Several other implementations of highly excited coupled cluster have been published so far, e.g. [1-4].
We focus here on the calculation of the residuals, which is the time determining step for the solution of coupled cluster equations. The key step with respect to efficiency is the implementation of the tensor contraction which is used for this calculation. We illustrate our approach based on matrix multiplication combined with an optimized rearranging of tensor entries [5].
In addition, we implemented a new method for the factorization of the expressions for the residuals [6]. Factorization here means the definition of a sequence of binary tensor contraction operations for the evaluation of these expressions. This includes the choice of the contractions to be carried out – in particular the order of the factors in each product –, the addition of compatible tensors before contraction, and the identification of reusable intermediates. All these steps are treated simultaneously as a coupled optimization problem. This optimization is carried out by a genetic algorithm.
We also show exemplary timings and analyze the performance of different program parts.

Literature:

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[6] M. Hanrath and A. Engels-Putzka, *"The (Highly Excited) Coupled Cluster Factorization Problem: A Genetic Approach"*, manuscript in preparation