Tensor decomposition in post-HF methods

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In this presentation details on the implementation and algorithm of the tensor decomposition technique for post-HF methods are presented (see contributed talk by Auer, Hamaekers and Schneider).



In typical applications of the tensor decomposition technique the time determining step in the original algorithm that was caused by processing highly-dimensional quantities vanishes and the actual tensor decomposition becomes dominant. If the decomposition is to be applied to quantities like the two-electron integrals or amplitudes special strategies have to be applied.



In this contribution we discuss details of the decomposition algorithm and examples for the decomposition of several quantities in post-HF methods. Furthermore, various strategies for the implementation of Coupled-Cluster methods using tensor decomposition are discussed.