Approximate coupled cluster models based on tensor decomposition techniques

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In this talk, recent advances in the development of approximate coupled cluster models based on tensor decomposition techniques will be outlined. In particular, we will focus on high-level methods, namely coupled-cluster method with single, double, and triple excitations (CCSDT) [6, 7] and CCSDT(Q) perturbative correction [1]. For the coupled-cluster triple and quadruple amplitudes tensor we employ the Tucker compression [8] format, for example

$$t_{ijk}^{abc} = t_{XYZ}\, U_{ia}^{X}\, U_{jb}^{Y}\, U_{kc}^{Z}, \tag{1}$$

where the quantities U_{ia}^{X} are obtained from higher-order singular value decomposition (HOSVD) of an approximate triple amplitudes tensor [2]. The central tensor t_{XYZ} is obtained as a result of the coupled-cluster iterations [3, 4]. The efficiency of the method relies on the fact that the optimal size of the SVD subspace (the length of the summation over X, Y, Z) sufficient to obtain a constant relative accuracy in the correlation energy scales linearly with the size of the system. Combined with proper factorization of the coupled-cluster equations this leads to N^6 scaling of the computational costs of the SVD-CCSDT method, compared with the N^8 scaling for the conventional (uncompressed) CCSDT. The (Q) correction can be evaluated with N^7 cost [5]. The method is chemically accurate and even more demanding levels of accuracy, such as 0.1 kJ/mol, can be obtained with a reasonable size of the SVD subspace.

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