Low-rank factorization of electron integral tensors and its application in electronic structure theory

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In this presentation, we will try to make some connections between graph theory and some post-Hartree-Fock methods with the purpose of finding a better way to reduce the cost of the expensive tensor contractions. As our first try, we apply the reverse Cuthill-McKee (RCM) algorithm to transform the two-electron integral tensors to their block diagonal forms. By further applying the Cholesky decomposition (CD) on each of the diagonal blocks, we are able to represent the high-dimensional two-electron integral tensors in terms of permutation matrices and low-rank Cholesky vectors. This representation facilitates the low-rank factorization of the high-dimensional tensor contractions in post-Hartree-Fock calculations. Here, we discuss the second-order Møller-Plesset (MP2) method and linear coupled-cluster model with doubles (L-CCD) as examples to demonstrate the efficiency of this technique in representing two-electron integrals in a compact form.