Title:

Performance Analysis of Diverse Coulomb and Exchange Matrix Algorithms

Abstract:

Efficient computation of the Coulomb (J) and Exchange (K) matrices is one of the most important aspects required for an electronic structure theory code, as the J and K matrices appear in many important quantum chemical methods such as Hartree-Fock (HF) and Density Functional Theory (DFT). Due to their importance, a significant number of algorithms exist for performant construction of the J and K matrices. Recently, a number of J and K build algorithms, such as the Linear Exchange (LinK) algorithm [1] for K matrix construction and the Continuous Fast Multipole Method (CFMM) [2] and integral-direct Density-Fitted HF (DF-HF) [3] methods for J matrix construction, have been programmed into the popular Psi4 code. These J and K algorithms were analyzed for performance and compared against both each other and the integral-direct combined JK build algorithm. For these different JK construction algorithms, scaling orders and algorithmic prefactors were determined using a variety of molecular systems. Additionally, the parallel efficiency of these algorithms were determined using said systems. The resulting analysis provides significant insight into the efficacy and performance characteristics of the different J and K construction algorithms tested.

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[2] White, C. A.; Johnson, B. G.; Gill, P. M. W.; Head-Gordon, M. Chem. Phys. Lett. 1994, 230, 8–16.
[3] Weigend, F. Phys. Chem. Chem. Phys. 2002, 4, 4285–4291.