Attacking the Strong and Weak Scaling Limits in Linear Scaling Hybrid Density Functional Theory

Robert A. DiStasio Jr.

Department of Chemistry and Chemical Biology

Cornell University

Email: distasio@cornell.edu

Abstract:
Hybrid density functional theory (DFT) represents a quite favorable balance between accuracy and cost, and has therefore become the de facto standard in quantum chemistry. However, the steep computational cost associated with a cubic-scaling reciprocal-space evaluation of the exact-exchange energy has largely hindered the widespread use of hybrid DFT in the condensed phase. By utilizing a local representation of the occupied space, we have developed a formally exact and linear-scaling algorithm that exploits the real-space sparsity in the exact-exchange interaction by rigorously treating all overlapping orbital pairs. In this work, we present a series of theoretical developments and algorithmic improvements which drastically reduce the time to solution and take us one step closer to routine hybrid DFT-based ab initio molecular dynamics simulations of large-scale condensed-phase systems. In particular, we will focus on: (i) novel preconditioning techniques to speed up the computation, (ii) game and graph theoretical methods to improve the workload imbalance, (iii) sparse and asynchronous data transfer to mitigate the communication cost, and (iv) extensive code optimization/vectorization to efficiently utilize current- and next-generation architectures.