Abstract Submitted
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Accelerating the Computation of Hartree-Fock Exchange using Recursive Bisection[1] IVAN DUCHEMIN, FRANCOIS GYGI, University of California Davis — The high computational cost of Hartree-Fock exchange currently limits the use of hybrid density functionals in First-Principles Molecular Dynamics (FPMD) applications. Efficient algorithms are essential for large-scale electronic structure calculations. We present a parallel implementation based on a recursive bisection algorithm [1] that allows one to reduce the number of significant exchange integrals with controlled accuracy. By adjusting the threshold of truncation of wavefunctions, the calculation is accelerated by a factor of up to 6 for a 32-molecule simulation of water. The accuracy of the truncation can be progressively adjusted during self-consistent iterations for optimal acceleration. We analyze the error in ionic forces as a function of the truncation threshold. The approach is demonstrated in a molecular dynamics simulation of liquid water using the PBE0 hybrid exchange-correlation functional.

[1] F. Gygi, Compact Representations of Kohn-Sham Invariant Subspaces, Phys. Rev. Lett. 102, 166406 (2009).

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