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Enabling Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics in Large-Scale Condensed-Phase Systems JUNTENG JIA, Cornell University, ALVARO VAZQUEZ-MAYAGOITIA, Argonne National Laboratory, ROBERT A. DISTASIO JR., Cornell University, CORNELL UNIVERSITY/ARGONNE NATIONAL LABORATORY COLLABORATION — Hybrid density functional theory (DFT) provides an accurate and reliable quantum mechanical model for studying condensed-phase systems. However, this accuracy is often accompanied by a prohibitively large computational cost associated with evaluating the exact exchange (E_{xx}) energy and corresponding orbital-dependent potential. In this work, we report some of our recent theoretical and algorithmic developments that significantly reduce the time to solution in condensed-phase hybrid DFT on modern supercomputer architectures. By utilizing maximally localized Wannier functions (MLWFs) for the occupied orbitals, we formally reduce the computational scaling to $O(N)$ in the system size. By devloping novel preconditioning techniques in conjunction with extensive code optimization/vectorization, we achieve an additional order of magnitude boost in performance when migrating from BG/Q to KNL during the solution of the Poisson equation (the computational cornerstone of our E_{xx} algorithm). A novel task-based distribution scheme that we have recently developed to minimize communication overhead and maximize load balance will also be discussed as a potential strategy for ensuring favorable scalability and portability of our algorithm to future petascale architectures.

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