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Optimization the localized orbitals in nearly O(N) electronic structure methods QINGZHONG ZHAO, WENCHANG LU, JERRY BERNHOLC, North Carolina State University — By using localized orbitals that are *variationally optimized* for each system, it is possible to evaluate the DFT total energy $O(N)$steps. However, the convergence of such methods is often impractically slow. We found it advantageous [1] to use a small, but larger than the minimum, number of non-orthogonal orbitals. These orbitals vanish beyond a fixed but fairly large localization radius around each atom. Parallelized diagonalization is used to accelerate convergence and the scaling remains nearly linear for up to 2000-3000 atoms. However, the localization approximation resulted in the total energy somewhat above the DFT limit. We show that by adding supplementary short-range orbitals, the true DFT limit is reached and the convergence properties improve significantly. Furthermore, the low-lying conduction states become sufficiently accurate for the description of Green's functions entering non-linear calculations of electron transport, which utilize this compact basis to reach very large system sizes. We will discuss both scalability issues and example applications during the talk. 1. J.-L. Fattebert and J. Bernholc, Phys. Rev. B 62, 1713 (2000).

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